APPLICATIONS OF DYNAMIC PROGRAMMING TO PROCESS ENGINEERING

by

LIEN-CHENG SU

B. S., National Taiwan University, 1955

A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1967

Approved by:

Liang-Tseng Fan

Major Professor

ACKNOWLEDGMENTS

The author wishes to express his sincere appreciation to Dr. Liang-tseng Fan for his constant enthusiasm and advice and for helpful guidance throughout the process of this work; Drs. Larry E. Erickson and Ching-lai Hwang for reading the manuscript; William H. Honstead, Head of the Department of Chemical Engineering, for his assistance and encouragement; the Kansas State University Computing Center for the use of their facilities; Kansas State Water Resources Research Institute and the Office of Saline Water for their financial assistance.

TABLE OF CONTENTS

CHAPTER I

INTRODUCTION

1. THE CONCEPT OF OPTIMIZATION

In recent years, chemical engineers have become increasingly concerned with the problems of choosing the design and operating variables of chemical plants such that some performance criteria are optimized. The intensive competition in the industry in general and in the chemical process industry in particular necessitates the improvement of technologies, since even marginal savings in production costs may be of vital importance in this competitive community. The act of optimization is essentially that of designing the most economical system of equipment and obtaining the best performance either under given conditions or subjected to certain restrictions.

A single optimization problem corresponds to the seeking of the extreme value of a function by differential calculus. But it is often the case that the optimal problems in engineering and industry cannot be solved by direct applications of conventional methods of optimization. Various schemes more sophisticated than the conventional methods have been proposed. Among them are the maximum principle, and dynamic programming.

2. THE FEATURES OF DYNAMIC PROGRAMMING

Dynamic programming provides a powerful tool for solving multistage decision processes, which arise in various fields. It is based upon the principle of optimality and employs the techniques of invariant imbedding [1, 2]. The concept upon which the dynamic programming technique is based is a new and versatile mathematical tool for the treatment of many novel and interesting problems.

Because of the simplicity and versatility of the principle of optimality, the method of dynamic programming can be used to deal with a process for which the transformation or transition at each stage is too complex to be expressed explicitly and analytically. Application of this principle also guarantees that the decision made at each stage is the best one in light of the entire process. While the number of stages in a process may be numerous, a small number of decisions are usually involved at each stage, and, with the aid of modern computers, one can often easily solve a multistage decision problem by using dynamic programming. A continuous process can also be optimized using dynamic programming by treating the process as one with a large number of infinitesimal stages.

3. THE APPLICATIONS OF DYNAMIC PROGRAMMING

Dynamic programming has been applied extensively to solve various practical and theoretical problems. Aris [3] has written a book dealing specifically with chemical reactor design. He has also written two other books related to the applications of dynamic programming [4, 5]. Roberts [6] has made optimal catalyst replacement studies. Aris et al. [7] studied optimum crosscurrent extraction. Rudd [8] has investigated a reliability problem in chemical system design and the optimal allocation of limited resources. A model for the optimization of countercurrent flow processes has been developed by Dranoff et al. [9]. Mitten and Nemhauser [10] applied the dynamic programming technique to determine the optimal design of a process consisting of a sequence of heterogeneous stages. Optimization methods applicable for processes with bypass and recycle streams have also been developed [11].

4. THE ALGORITHM OF DYNAMIC PROGRAMMING AND THE PRINCIPLE OF OPTIMALITY

The essential notions of dynamic programming are linked to a serial structure. It is of the nature of serial optimization. Its cornerstone is the principle of optimality founded by Bellman [1]. It states that "An optimal policy has the property that whatever the initial state and initial decisions are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision."

The mathematical transliteration of this principle yields a new class of functional equations, and the mathematical viewpoint developed in treating these problems enables us to approach some classical as well as new problems.

5. THE INVERSE PRINCIPLE OF OPTIMALITY

If we stipulate the output x of the sequential process of Fig. 1, but not the input x_{N+1}, then there is an inverse principle of optimality for such a process, provided the stage transformation may be inverted. The inverse of the transformation at stage n can be written as

$$x_{n+1} = \bar{T}_n(x_n : \theta_n) , \qquad n = 1, 2, \ldots, N-1 .$$

The inverse principle is stated as follows [5]:

In a sequential process, the optimal policy for a fixed final and free initial state has the property that whatever the final state and decision may be, the proceeding decisions constitute an optimal policy with respect to the state resulting from them.

6. MULTISTAGE DECISION PROCESSES

A typical multistage stagewise process is shown in Fig. 1 where x_n is a state vector which represents the state variables from stage n, and θ_n is a vector which stands for the decision variables in stage n. Note that the

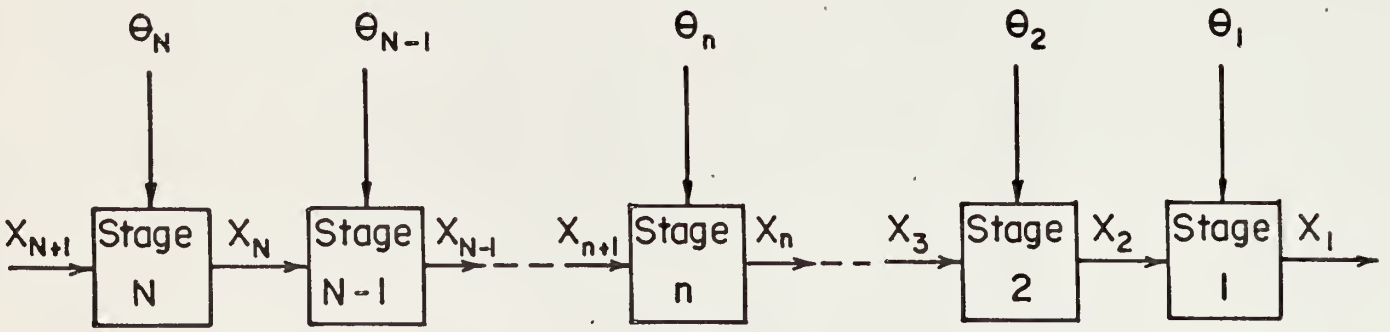


Fig. 1. A typical multi-stage process (backward numbering).

stages have been numbered in the backward direction. They can equally well be numbered in the forward manner, which ever is more convenient.

If these stages are series of continuous flow stirred tank reactors (CSTR system), then the state variables may be concentrations of the various species--reactants and/or products. Decision variables of a CSTR system may be the temperature and pressure of the reaction mixture, but the specification of a decision variable is quite arbitrary. It could be the flow rate or equivalently the residence time of each stage.

The function of each stage is to transform the state variables from the input state to the output state. This transformation can generally be expressed as

$$x_n = T_n(X_{n+1};\ \theta_n) , \qquad n = N,\ N-1,\ldots,\ 2,\ 1 . \tag{1}$$

Equation (1) is in vector form. If there are s state variables and one decision variable, equation (1) can be written as

$$x_{i,n} = T_{i,n}(x_{1,n+1},\ x_{2,n+1},\ldots,\ x_{s,n+1},\ \theta_n) , \tag{2}$$

$$i = 1,\ 2,\ldots,\ s$$

$$n = N,\ldots,\ 2,\ 1 .$$

The objective of optimization is to seek a set of admissible values of $\theta_1,\ \theta_2,\ldots,\ \theta_N$ so that a desired performance criterion or a return function which is usually called an objective function is maximized (or minimized). The characteristic feature of a multistage decision process is that there is an interval profit or return associated with each stage of the process and the objective function can be expressed as the summation of the interval profits

$$S(x_{N+1};\ \theta_N,\ldots,\ \theta_1) = \sum_{n=N}^{1} g_n(x_{n+1};\ \theta_n)\ . \tag{3}$$

The value of the objective function depends on the initial state and a sequence of decisions $\theta_N,\ldots,\ \theta_1$. If we represent the maximum return function by $f_N(x_{N+1})$, then

$$\begin{aligned} f_N(x_{N+1}) &= f_N(x_{1,N+1},\ x_{2,N+1},\ldots,\ x_{s,N+1}) \\ &= \max\ S(x_{N+1};\ \theta_N,\ldots,\ \theta_1) \\ &= \max_{\theta_n} \sum_{n=N}^{1} g_n(x_{n+1};\ \theta_n)\ . \end{aligned} \tag{4}$$

Thus, in general, $f_n(x_{n+1})$ is the maximum return obtainable from the operation of an n-stage process if an optimal policy is followed starting with the initial state x_{n+1}.

If there is one decision variable in each stage, equation (4) expresses an N-dimensional optimization problem because this problem must be optimized with respect to all the N decision variables. The dynamic programming technique treats this problem as N one-dimensional problems. For a one-stage process, equation (4) becomes

$$f_1(x_2) = \max_{\theta_1} g_1(x_2;\ \theta_1)$$

which is the simplest optimization problem among the sequence of problems for n = 1, 2,..., N. The other members of this sequence can be obtained by writing equation (4) in the form:

$$f_n(x_{n+1}) = \max_{\theta_n}\ \max_{\theta_{n-1}}\ \ldots\ \max_{\theta_1} \left[g_n(x_{n+1};\ \theta_n) + \ldots + g_1(x_2;\ \theta_1)\right] \tag{5}$$

or

$$f_n(x_{n+1}) = \max_{\theta_n} \left\{ g_n(x_{n+1};\ \theta_n) + \max_{\theta_{n-1}} \ \ldots \ \max_{\theta_1} g_{n-1}(x_n;\ \theta_{n-1}) \right.$$

$$\left. + \ldots + g_1(x_2;\ \theta_1) \right\} . \qquad (6)$$

The expression

$$\max_{\theta_{n-1}} \ \ldots \ \max_{\theta_1} \left[g_{n-1}(x_n;\ \theta_{n-1}) + \ldots + g_1(x_2;\ \theta_1) \right]$$

stands for the maximum return (the objective function) from an (n-1)-stage process with initial stage x_n. Hence, we can also write

$$f_{n-1}(x_n) = \max_{\theta_{n-1}} \ \ldots \ \max_{\theta_1} \left[g_{n-1}(x_n;\ \theta_{n-1}) + \ldots + g_1(x_2;\ \theta_1) \right] \qquad (7)$$

Thus, equation (6) can be simplified to

$$f_n(x_{n+1}) = \max_{\theta_n} \left[g_n(x_{n+1};\ \theta_n) + f_{n-1}(x_n) \right] \qquad (8)$$

or

$$f_n(x_{n+1}) = \max_{\theta_n} \left[g_n(x_{n+1};\ \theta_n) + f_{n-1}(T(x_{n+1};\ \theta_n)) \right] .$$

This is the so-called functional equation of dynamic programming. It gives a recursion relationship between an N stage process and an N-1 stage process. The solution of the functional equation yields the value of the maximum return and the corresponding optimal policy, which belongs to the set $\{\theta_n\}$.

If we consider the process with stages numbered in the forward order (see Fig. 2), the transformation equation is usually in the form of

$$x_n = T_n(x_{n-1};\ \theta_n) , \qquad n = 1, 2, \ldots, N ,$$

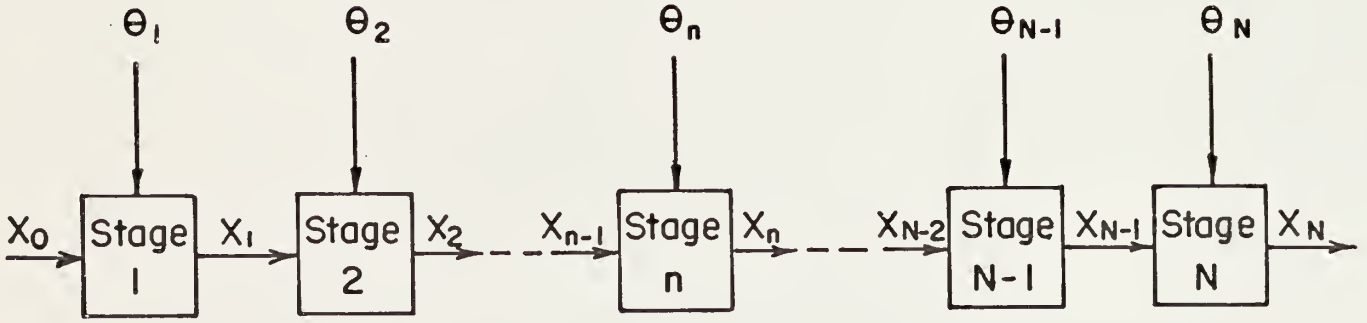


Fig. 2. A typical multi-stage process (forward numbering).

and the objective of maximum return function is

$$f_N(x_0) = \max S(x_0; \theta_1, \theta_2, \ldots, \theta_N)$$

$$= \max_{\{\theta_n^n\}} \sum_{n=1}^{N} g_n(x_{n-1}; \theta_n) .$$

Therefore, the functional equation can be written as

$$f_N(x_0) = \max_{\theta_1} \left\{ g_1(x_0; \theta_1) + f_{N-1}(x_1) \right\} .$$

Another form for expressing the transformation equation is*

$$x^n = T^n(x^{n-1}; \theta^n) , \qquad n = 1, 2, \ldots, N$$

and the objective or maximum return function is

$$f^N(x^0) = \max S(x^0; \theta^1, \theta^2, \ldots, \theta^N)$$

$$= \max_{\{\theta^n\}} \sum_{n=1}^{N} G^n(x^{n-1}; \theta^n)$$

so that the functional equation takes the form

$$f^N(x^0) = \max_{\theta^1} \left\{ G(x^0; \theta^1) + f^{N-1}(x^1) \right\} .$$

Another way of interpreting the principle of optimality is imbedding a smaller system into a bigger system as shown in Fig. 3. The functional equation is of the form

---

*The superscripts denote the stage number. The power of n is represented by putting n outside of the parenthesis.

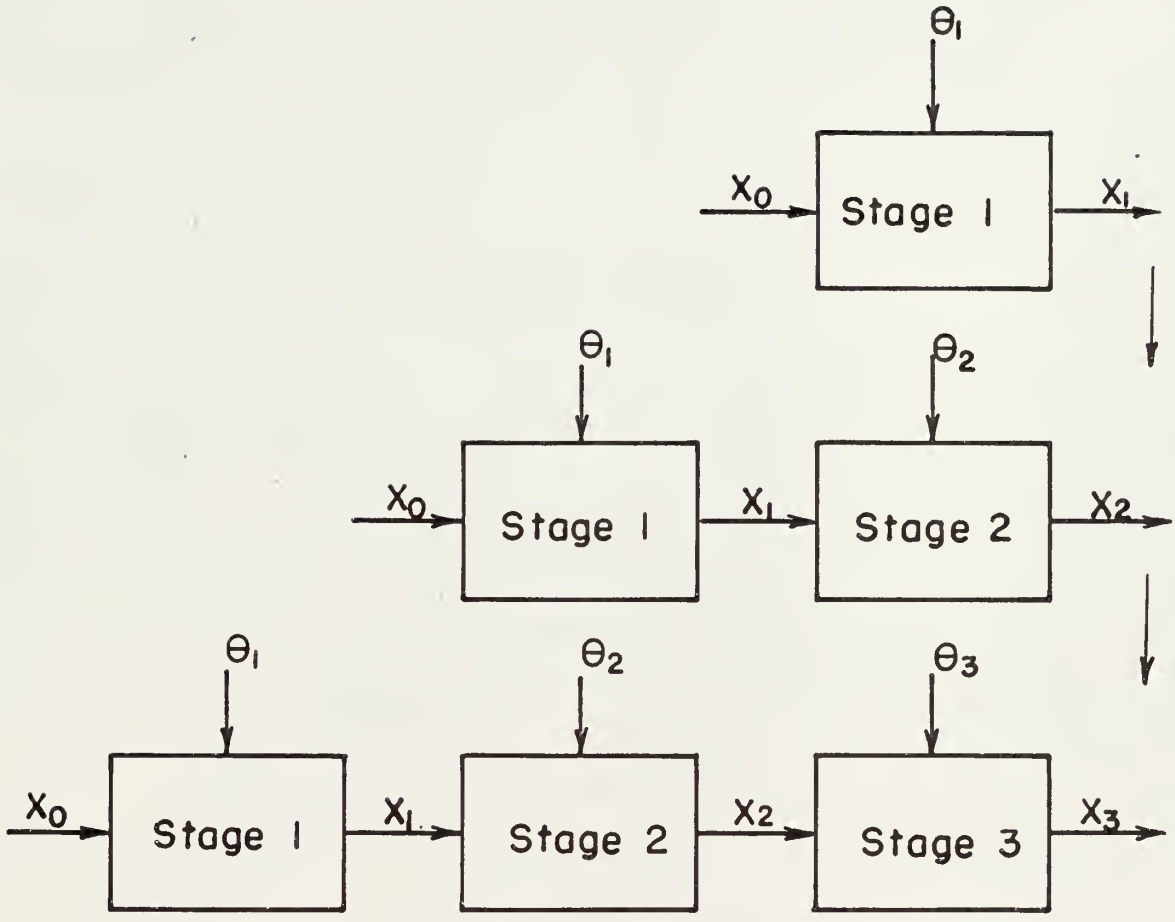


Fig. 3. A schematic diagram showing the imbedding of a smaller system into a bigger system. The arrows indicate the direction of imbedding.

$$f_1(x_o) = \max_{\theta_1} g_1(x_o; \theta_1)$$

$$f_2(x_o) = \max_{\theta_1} g_1(x_o; \theta_1) + f_1(T_1(x_o; \theta_1))$$

and in general

$$f_N(x_o) = \max_{\theta_1} \left\{ g_1(x_o; \theta_1) + f_{N-1}(T_{N-1}(x_{N-2}; \theta_{N-1})) \right\}$$

Generally speaking, the evaluation of the functional equation seldom appears in an analytical form. Instead, the equation is evaluated by numerical methods on a high speed computer.

7. THE ADVANTAGES AND DISADVANTAGES OF DYNAMIC PROGRAMMING

Dynamic programming provides a new tool for solving problems which were formerly considered too complicated to be solved. It can be applied to a series of stages which have different operating and state variables at each stage. Furthermore, by the use of the principle of optimality, a chemical process can be separated into different segments (subprocesses) and each segment can be optimized by a different technique. Another important feature of dynamic programming lies in its ability to handle any kind of constraints. Many types of constraints cause trouble when other techniques are used [12].

The principle disadvantage of dynamic programming is the problem of high dimensionality. Since we imbed a whole family of decisions, enormous time and space are required, and the available memory in a modern computer still limits the use of the dynamic programming technique to systems of several variables. This is the so-called "curse of dimensionality" [1]. Any reduction in dimensionality achieved by the use of mathematical knowledge will

save tremendously in computational cost.

Another disadvantage of dynamic programming is that in using it to optimize continuous processes it leads to a set of partial differential equations. However, it is often possible to convert this set of partial differential equations into a system of finite difference equations. Thus, the method of dynamic programming can be used to optimize continuous processes [4].

A third disadvantage of dynamic programming is that it cannot be applied easily to processes in which the optimum conditions at any stage can be disturbed by conditions at a following stage. This is a rather serious limitation if we consider the various feedback and countercurrent operations which are often employed in the chemical and petroleum industries [12].

8. THE OBJECTIVES AND SCOPE OF THIS WORK

In this work, a comprehensive study of the theories and applications of dynamic programming together with some techniques for reducing dimensionality are presented. The wide applicability of dynamic programming in optimizing multistage decision processes is illustrated by using it to optimize several process engineering problems.

References

1. Bellman, R., "Dynamic Programming," Princeton University Press, New Jersey, 1957.

2. Bellman, R. and S. E. Dreyfus, "Applied Dynamic Programming," Princeton University Press, New Jersey, 1962.

3. Aris, R., "The Optimal Design of Chemical Reactors," Academic Press, New York, 1961.

4. Aris, R., "The Discrete Dynamic Programming," Blaisdell, New York, 1964.

5. Aris, R., "Dynamic Programming," Socony Mobil Oil Company, Inc., Field Research Laboratory, Dallas, Texas, 1963.

6. Roberts, S. M., "Dynamic Programming in Chemical Engineering and Process Control," Academic Press, New York (1964).

7. Aris, R., D. F. Rudd and N. R. Amundson, "On Optimum Crosscurrent Extraction," Chem. Eng. Sci., Vol. 12, 88-97 (1960).

8. Rudd, D. F., "Reliability Theory in System Design," I & EC Fundamentals, Vol. 7, No. 2, 138 (1962).

9. Dranoff, J. S., L. G. Mitten, W. F. Stevens and L. A. Wanniger, "Application of Dynamic Programming to Countercurrent Flow Processes," Operations Research, Vol. 9, No. 3, 288-401 (1961).

10. Mitten, L. G. and G. L. Nemhauser, "Multistage Optimization," Chem. Eng. Progr., Vol. 59, No. 1, 52-60 (1963).

11. Nemhauser, G. L., "Introduction to Dynamic Programming," John Wiley and Sons, Inc., New York, 1966.

12. Lee, E. S., "Optimum Design and Operation of Chemical Processes," Industrial and Engineering Chemistry, Vol. 55, No. 8 (1963).

CHAPTER II

GENERAL DESCRIPTIONS AND APPLICATIONS TO SIMPLE PROCESSES

1. COMPUTATIONAL SCHEME FOR THE FUNCTIONAL EQUATION [1].

As stated in Chapter I, the functional equation is of the form

$$f_n(x_{n+1}) = \max_{\theta_n} \left\{ g_n(x_{n+1};\ \theta_n) + f_{n-1}(x_n) \right\}.$$

for an n-stage process starting with an initial state x_{n+1} as shown in Fig. 1 (backward numbering system) in Chapter I.

The significance of the functional equation is that the optimal decision at stage n is so chosen that the sum of $f_{n-1}(x_n)$ and $g_n(x_{n+1};\ \theta_n)$ is maximized. Since the states of the intermediate stages are unknown before the problem is completely solved, the functional equation cannot become immediately useful in solving an n-stage optimization problem. The so-called imbedding technique is carried out in two steps to establish the recurrence relationships. The first step is to construct a table for each stage relating the corresponding optimal decision to the objective function for various values of the state variable entering each stage. The second step is to determine the optimal policy for the whole process by means of the table entry technique utilizing all the optimal tables constructed [2].

In constructing the optimal tables, the computation is initiated with the last stage, proceeding backwards to the initial stage. In each step of tabulation, the stage for which the optimal table is to be tabulated is regarded as the initial stage. For example, if we are constructing the optimal table for stage n, it is taken as the initial stage, whereas all the downstream stages are included in an (n-1)-stage process for which the

capacities of only about 3.2×10^4 locations, three-dimensional problems cannot be solved routinely. This is known as the dimensionality difficulty of the dynamic programming approach.

It is worthwhile to mention that there is also a functional equation of the form [3]

$$f_n(x_{n+1}) = \max_{\theta_n} \left\{ g_n(x_{n+1};\ \theta_n) \cdot f_{n-1}(x_n) \right\} .$$

A simple example of its use is to divide a distance ℓ into n parts in such a way that the product of the n parts is a maximum. In this case, we let $f_n(\ell)$ be the maximum attainable product, x be the length of the first subdivision, and $(\ell - x)$ be the length of the remaining (n-1) parts. Then, the functional equation takes the form [4]

$$f_n(\ell) = \max_{0 \leq x \leq \ell} \left\{ x f_{n-1}(\ell - x) \right\} .$$

2. ILLUSTRATIVE PROBLEMS IN ENGINEERING

EXAMPLE 1, ALLOCATION OF PRODUCTION LEVEL.

Let us consider a typical linear programming problem in which N grades of paper are produced on a paper machine. Due to the restrictions on the raw materials, not more than a_i tons of grade i can be produced in a week.

Let

x_i = number of tons of grade i produced in the week

b_i = number of hours required to produce a ton of grade i

P_i = net profit per ton of grade i.

The problem in hand can be stated as

$$0 \leq x_i \leq a_i$$

$$\sum_{i=1}^{N} b_i x_i \leq c = \text{total production hours}$$

$$\max S = \max P(x_1, \ldots, x_N) = \max \sum_{i=1}^{N} P_i x_i .$$

We shall consider this problem as an N-stage process with one decision variable at each stage. According to the notion of dynamic programming, we define a maximum return function

$f_N(c)$ = maximum return obtainable from the N-stage process with c production hours per week.

so that

$$f_N(c) = \max_{\{x_i\}} P(x_1, \ldots, x_N) = \max_{\{x_i\}} \sum_{i=1}^{N} P_i x_i$$

where $\{x_i\}$ indicates a series of decision variables $x_1, \ldots, x_N$.

For ease of discussion, let us change the inequality constraint to the following equality constraint.

$$\sum_{i=1}^{N} b_i x_i = c .$$

This is a typical allocation problem [1]. Many other types of allocation problems can be found in any book treating dynamic programming [5, 6]. We wish to allocate the total of c working hours to produce N-different grades of papers in an optimal way.

For a one-stage process, i.e. only one grade of paper is produced, the maximum return becomes

$$f_1(c) = \max_{0 \leq x_1 \leq a_1} P_1 x_1 = P_1 \frac{c}{b_1}$$

with $0 \leq \frac{c}{b_1} \leq a_1$.

For a two-stage process, the maximum return $f_2(c)$ is written as

$$f_2(c) = \max_{0 \leq x_2 \leq a_2} [P_2 x_2 + f_1(c - b_2 x_2)] .$$

It is understood that whatever the amount of c which has already been allocated to the second stage, the remaining amount $c - b_2 x_2$ must be used in an optimal way for the remaining one-stage process.

Extending this notion, we see that whatever the amount of c which has already been allocated to the N-th stage for an N-stage process, the remaining amount $c - b_N x_N$ must be allocated in the optimal way for the remaining (N-1)-stage process.

Thus, the maximum return for an N-stage process is

$$f_N(c) = \max_{0 \leq x_N \leq a_N} P_N x_N + f_{N-1}(c - b_N x_N) .$$

It can be seen that this algorithm can be extended to the multidimensional case.

For illustration, let us consider the case of N = 2 and

$$x_1 \leq 500, \qquad x_2 \leq 250 , \tag{1}$$

$$0.2\, x_1 + 0.4\, x_2 \leq 140 , \tag{2}$$

$$P(x_1, x_2) = 20\, x_1 + 45\, x_2 . \tag{3}$$

Equation (2) can be written as

$$x_1 + 2x_2 \leq 700 = c . \tag{4}$$

Note that $a_1 = 500$, $a_2 = 250$, $b_1 = 1$, $b_2 = 2$, $P_1 = 20$ and $P_2 = 45$.

The maximum return for a one-stage process can be rewritten as

$$f_1(c) = \max_{0 \leqslant x_1 \leqslant a_1} p_1 x_1(c) \ . \tag{5}$$

Due to the constraint on x_1, the maximum return is

$$f_1(c) = p_1 \frac{c}{b_1} = 20c \ , \qquad c \leqslant a_1 = 500 \tag{6}$$

$$f_1(c) = 20\, a_1 = 10{,}000 \ , \qquad c \geqslant a_1 = 500 \ . \tag{7}$$

The optimal table with a grid value of $c = 100$ is given in Table 1.

The maximum return for a two stage process is

$$f_2(c) = \max_{0 \leqslant x_2 \leqslant a_2} [p_2 x_2(c) + f_1(c - b_2 x_2(c))] \ . \tag{8}$$

We define

$$r_2(c) = p_2 x_2(c) + f_1(c - b_2 x_2(c)) \ , \tag{9}$$

then it follows that

$$f_2(c) = \max_{x_2} r_2(c) \ . \tag{10}$$

Values of $r_2(c)$ with $c = 100$ is given in Table 2.

It is seen that $f_2(c) = 2250$ for $c = 100$. In a like manner, we can find $f_2(c)$ for other grid values of c, and the optimal table for the two-stage process is tabulated in Table 3.

It is concluded that the maximum return for the two-stage process will be \$15,250/week with an optimal allocation of production hours to produce 200 and 250 tons per week of grades 1 and 2 paper respectively. This

TABLE 1

OPTIMAL TABLE (ONE STAGE PROCESS)

c hr/week	$x_1 = \theta_1$ ton/week	$p_1 x_1$ \$/week	$f_1(c)$ \$/week
0	0	0	0
100	100	2,000	2,000
200	200	4,000	4,000
300	300	6,000	6,000
400	400	8,000	8,000
500	500	10,000	10,000
600	500	10,000	10,000
700	500	10,000	10,000

TABLE 2

VALUES OF $r_2(c)$ FOR TWO STAGE PROCESS

c hr/week	b_2x_2 hr/week	$x_2 = \theta_2$ ton/week	p_2x_2 $/week	$f_1(c-b_2x_2)$ $/week	$r_2(c)$ $/week
100	0	0	0	2,000	2,000
100	20	10	450	1,600	2,050
100	40	20	900	1,200	2,100
100	60	30	1,350	800	2,150
100	80	40	1,800	400	2,200
100	100	50	2,250	0	2,250

TABLE 3

OPTIMAL TABLE (TWO STAGE PROCESS)

c hr/week	$x_2 = \theta_2$ ton/week	p_2x_2 $/week	$f_1(c-b_2x_2)$ $/week	$f_2(c)$ $/week
0	0	0	0	0
100	50	2,250	0	2,250
200	100	4,500	0	4,500
300	150	6,750	0	6,750
400	200	9,000	0	9,000
500	250	11,250	0	11,250
600	250	11,250	2,000	13,250
700	250	11,250	4,000	15,250

example is essentially that given by Lee [7].

EXAMPLE 2. DIRECTED NETWORK PROBLEM

(a) Both ends fixed (boundary value problem)

In Fig. 1, the circles represent the nodes, and the numbers on the lines connecting nodes denote the distance between the nodes. Suppose that the problem is to look for the minimum length or the shortest path starting from left to right.

According to the classical method, all possibilities must be enumerated. But the enumeration of all the possibilities would be prohibitive for a large size problem. We work backwards employing the dynamic programming approach in the following.

Stage III

path	distance
1	1
2	10

There is no choice of path for each initial state.

Stage II (III)

path	distance
1	$6+1 = 7$
2	$7+10 = 17$
3	$10+1 = 11$
4	$9+10 = 19$

Paths 2 and 4 are eliminated from our consideration.

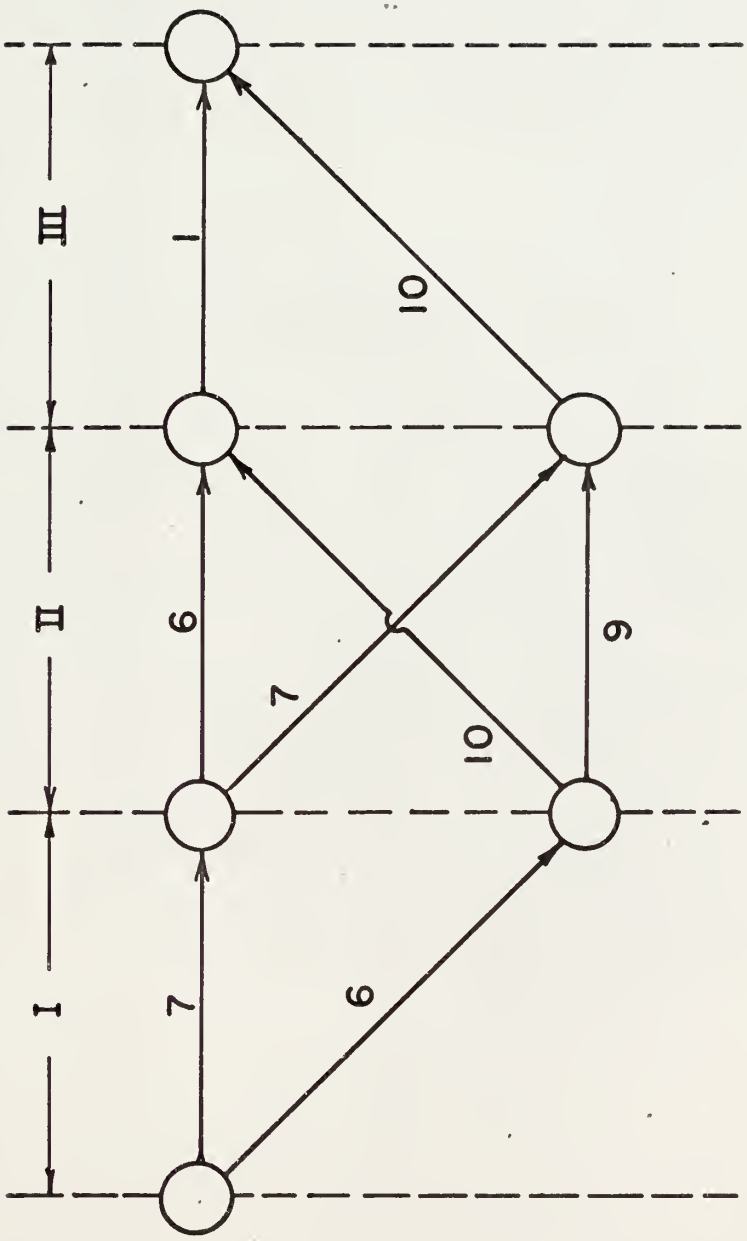


Fig. 1. Directed network with both ends fixed.

maximum values of the objective function denoted as $f_{n-1}[T_n(x_{n+1};\ \theta_n)]$ are already obtained and tabulated. By means of the functional equation and the optimal table of stage (n-1), we can obtain the optimal decision at stage n for each possible value of the state variable entering that stage. The decisions so obtained and the corresponding value of $f_n(x_{n+1})$ are listed in the table, which in turn is used to construct the optimal table for the preceding stage.

For comparison, we consider the computing time required for both the method of exhaustive search and dynamic programming. For a process with both ends free, there are $N(M)^N$ possible paths if there are N stages with M grid points of the state variable at each stage. Assuming that it takes approximately 10^{-4} seconds to compute one path, then the total computing time would be 5×10^9 years in the former case (N = 20, M = 10). But in the latter case, the number of computations is $(2N-1)M^2$ and it takes only 1 second and hence tremendous saving in computing time is obtained.

It may be noted that because we can compute the values of $f_n(x_{n+1})$ for only a finite number of admissible values of x_{n+1}, the methods of interpolation or extrapolation must be used to obtain the values of $f_n(x_{n+1})$ for those values of x_{n+1} which fall between two neighboring values of x_{n+1} listed in the optimal table.

The above computational procedure is only applicable to a one-dimensional multistage decision process, but this scheme can be extended to the multidimensional case. It is seen that the storage requirement of a computer increases exponentially with the dimensionality of the initial state variables. Usually, the storage requirement of a problem is about $(100)^s$ where s is the number of state variables. Since current computers have fast memory

Stage I (II & III)

path	distance
1	7+7 = 14
2	6+11 = 17

We see that the minimum distance is 14 with the path 7⟶6⟶1.

(b) Both ends free

We shall find the minimum distance starting from left to right by means of dynamic programming (Fig. 2).

Stage III

path	distance
1	1
2	4
3	10
4	3

Paths 2 and 3 are eliminated from our consideration.

Stage II(& III)

path	distance
1	6+1 = 7
2	7+3 = 10
3	10+1 = 11
4	9+3 = 12

Paths 2 and 4 are rejected.

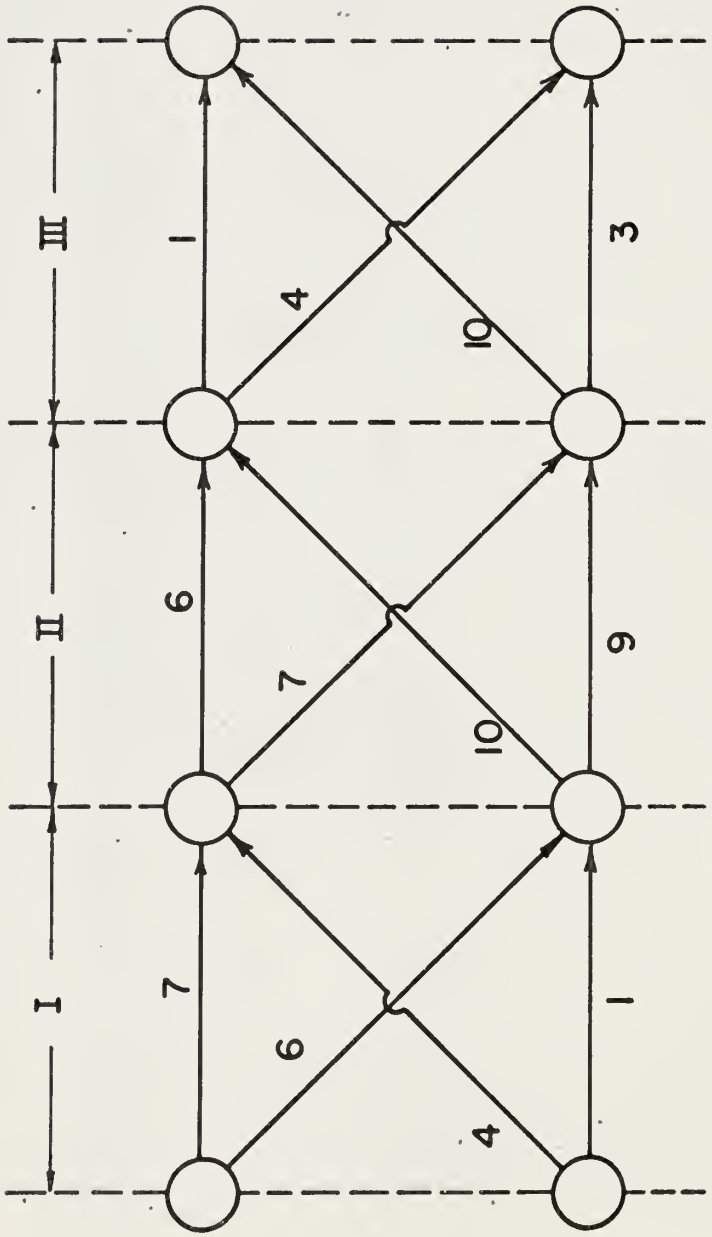


Fig. 2. Directed network with both ends free.

Stage I (II & III)

path	distance
1	7+7 = 14
2	6+11 = 17
3	4+7 = 11
4	1+11 = 12 .

We see that the minimum distance is 12 corresponding to the path 4⟶6⟶1.

(c) If the final state is fixed, it becomes a final value problem, whereas if the initial state is specified, it becomes an initial value problem. The computational scheme is essentially the same as that of cases (a) and (b).

EXAMPLE 3. ALLOCATION OF REACTOR VOLUMES IN A CSTR SYSTEM

Let us consider a liquid-phase chemical reaction between two immiscible reactants A and B. The reaction mechanism is

$$A + B \longrightarrow C + D$$

where C is miscible with A and D is miscible with B. The overall kinetics is assumed to be

$$-r_A = \frac{1}{V}\frac{dN_A}{dt} = kC_A C_B .$$

It is assumed that there is complete mixing in each reactor and that the rate is controlled by the chemical reaction only. In the above equation C_A and C_B are the concentrations of A and B in the completely mixed system.

The reaction is carried out in a sequence of three stirred tank reactors connected in series with equimolar feed of A and B flowing either cocurrently or countercurrently to achieve a prescribed degree of conversion. The process flow diagram is shown in Fig. 1a for the cocurrent flow system

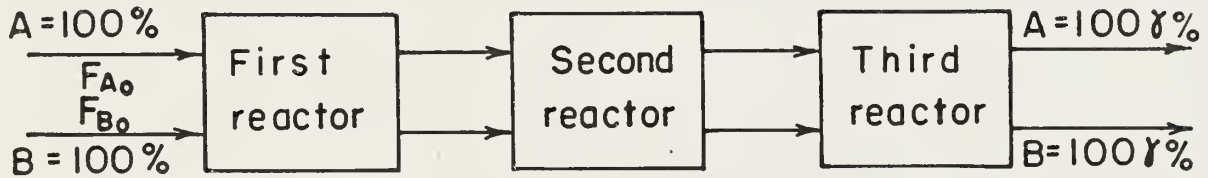


Fig. 1a. Schematic diagram of the two-phase cocurrent reactor system.

and in Fig. 1b for the countercurrent flow system. The volume of stage n (the nth reactor) can be obtained from the material balance as follows:

$$V^n(-r_A^n) = F_{AO}(x_A^n - x_A^{n-1})$$

$$V^n = \frac{F_{AO}(x_A^n - x_A^{n-1})}{-r_A^n}$$

$$= \frac{F_{AO}(x_A^n - x_A^{n-1})}{kC_{Ai}C_{Bi}(1-x_A^n)(1-x_B^n)}$$

with C_{Ai} and C_{Bi} defined as

$$C_{Ai} = \frac{F_{AO}}{\frac{F_{AO}}{C_{AO}} + \frac{F_{BO}}{C_{BO}}}$$

$$C_{Bi} = \frac{F_{BO}}{\frac{F_{AO}}{C_{AO}} + \frac{F_{BO}}{C_{BO}}}$$

where

F_{AO} = feed rate of A based on the inlet condition, lb-mole/sec.

F_{BO} = feed rate of B based on the inlet condition, lb-mole/sec.

k = specific rate constant, ft^3/sec. lb-mole,

C_{AO} : initial concentration of reactant A, lb-mole/ft^3,

C_{BO} : initial concentration of reactant B, lb-mole/ft^3,

x_A : degree of conversion of reactant A,

x_B : degree of conversion of reactant B.

For isothermal operation,

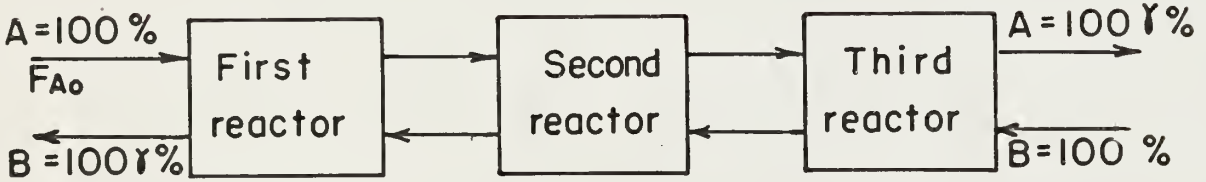


Fig. 1b. Schemetic diagram of the two-phase counter-current reactor system .

$$\frac{F_{AO}}{kC_{Ai}C_{Bi}}$$

is a constant.

For simplicity, we shall consider the case for which

$$\frac{F_{AO}}{kC_{Ai}C_{Bi}} = 1$$

and

$$F_{AO} = F_{BO} .$$

Furthermore, since pure A and pure B are fed to the system, we can write

$$x_A^n = x_B^n \tag{12a}$$

for the cocurrent system, and the equation

$$x_A^{n-1} + x_B^n = \text{final conversion} = \gamma \tag{12b}$$

holds for each stage in the case of countercurrent flow. Hence equation (11) can be rewritten as

$$V^n = \frac{x_A^n - x_A^{n-1}}{(1 - x_A^n)^2} \tag{13a}$$

for cocurrent flow and

$$V^n = \frac{x_A^n - x_A^{n-1}}{(1-x_A^n)(1-\gamma + x_A^{n-1})} \tag{13b}$$

for countercurrent flow.

The objective is to minimize the total reactor volume for a prescribed degree of conversion of reactant A by proper choices of conversion at stages 1 and 2 or equivalently by proper allocations of the reactor volume to individual reactors. That is,

$$\text{min. } S = \text{min. } \sum_{n=1}^{3} V^n , \qquad n = 1, 2, 3 .$$

We define conversion of reactant A at stage n-1 as the state variable, x_1^{n-1}, and the conversion of reactant A at the exit of stage n as the decision variable θ^n, i.e.

$$x_1^n = \theta^n . \tag{14}$$

Thus equation (13a) for the cocurrent system can be rewritten as

$$V^n = g_1(x_1^{n-1}; \theta^n) = \frac{\theta^n - x_1^{n-1}}{(1 - \theta^n)^2} , \qquad n = 1, 2, 3 . \tag{15a}$$

and the objective function becomes

$$\min S = \min \sum_{n=1}^{3} V^n$$

$$= \min_{\{\theta^n\}} \sum_{n=1}^{3} g_1(x_1^{n-1}; \theta^n) , \qquad n = 1, 2, 3 . \tag{16a}$$

Similarly, equation (13b) for the countercurrent system becomes

$$V^n = g_2(x_1^{n-1}; \theta^n) = \frac{\theta^n - x_1^{n-1}}{(1-\theta^n)(1-\gamma + x_1^{n-1})} , \tag{15b}$$

$$n = 1, 2, 3 .$$

and the objective function takes the form

$$\min S = \min \sum_{n=1}^{3} V^n$$

$$= \min_{\{\theta^n\}} \sum_{n=1}^{3} g_2(x_1^{n-1}; \theta^n) , \qquad n = 1, 2, 3 . \tag{16b}$$

Therefore, the functional equations of dynamic programming are as follows:

(A) Cocurrent system.

$$f_1(x_1^2) = \min_{\theta^3} \left\{ \frac{\theta^3 - x_1^2}{(1-\theta^3)^2} \right\} = \min_{\theta^3} g_1(x_1^2; \theta^3)$$

$$= \frac{\gamma - x_1^2}{(1-\gamma)^2}$$

for a one-stage process including stage 3 (the third reactor),

$$f_2(x_1^1) = \min_{\theta^2} \left\{ g_1(x_1^1; \theta^2) + f_1(x_1^2) \right\}$$

$$= \min_{\theta^2} \left\{ \frac{\theta^2 - x_1^1}{(1-\theta^2)^2} + f_1(x_1^2) \right\}$$

for a two-stage process including stage 2 (the second reactor) and stage 3,

$$f_3(x_1^0) = \min_{\theta^1} \left\{ g_1(x_1^0; \theta^1) + f_2(x_1^1) \right\}$$

$$= \min_{\theta^1} \left\{ \frac{\theta^1}{(1-\theta^1)^2} + f_2(x_1^1) \right\}$$

for a three-stage process including all reactors.

It is worth noting that

$$x_1^0 = 0 ,$$

$$x_1^3 = \theta^3 = \gamma .$$

(B) Countercurrent system.

$$f_1(x_1^2) = \min_{\theta^1} g_2(x_1^2; \theta^3)$$

$$= \min_{\theta^1} \left\{ \frac{\theta^3 - x_1^2}{(1-\theta^3)(1-\gamma + x_1^2)} \right\}$$

$$= \frac{\gamma - x_1^2}{(1-\gamma)(1-\gamma + x_1^2)}$$

for a one-stage process including stage 3 (the third reactor),

$$f_2(x_1^1) = \min_{\theta^2} \left\{ g_2(x_1^1; \theta^2) + f_1(x_1^2) \right\}$$

$$= \min_{\theta^2} \left\{ \frac{\theta^2 - x_1^1}{(1-\theta^2)(1-\gamma + x_1^1)} + f_1(x_1^2) \right\}$$

for a two-stage process including stage 2 (the second reactor) and stage 3,

$$f_3(x_1^0) = \min_{\theta^1} \left\{ g_2(x_1^0;\ \theta^1) + f_2(x_1^1) \right\}$$

$$= \min_{\theta^1} \left\{ \frac{\theta^1}{(1-\gamma)(1-\theta^1)} + f_2(x_1^1) \right\}$$

for a three-stage process including all reactors.

The block diagram representing these functional relationships is given in Fig. 2.

COMPUTATION AND RESULTS

The computations have been performed on an IBM 1620 computer. The computer symbols and program are given in Tables 1 and 2, and the computer flow diagram is shown in Fig. 3. For purposes of illustration optimal tables are given in Tables 3a, 3b, and 3c for the cocurrent system and Tables 4a, 4b, and 4c for the countercurrent system for a coarse grid. More exact values of the optimal reactor volume for each stage in both cases are listed in Table 5. The optimal total reactor volume is plotted as a function of the conversion of reactant A in Fig. 4.

It can be concluded that:

(1) The optimal volume of each stage is the same regardless of the conversion of reactant A in the countercurrent reaction system. The small variations in reactor volume allocation are due to the discretization error incurred by choosing a finite number of grid prints for computation.

(2) For the same degree of conversion of reactant A, the countercurrent flow reaction scheme is more economical than the cocurrent flow reaction scheme if we reglect the cost of separators for the countercurrent flow

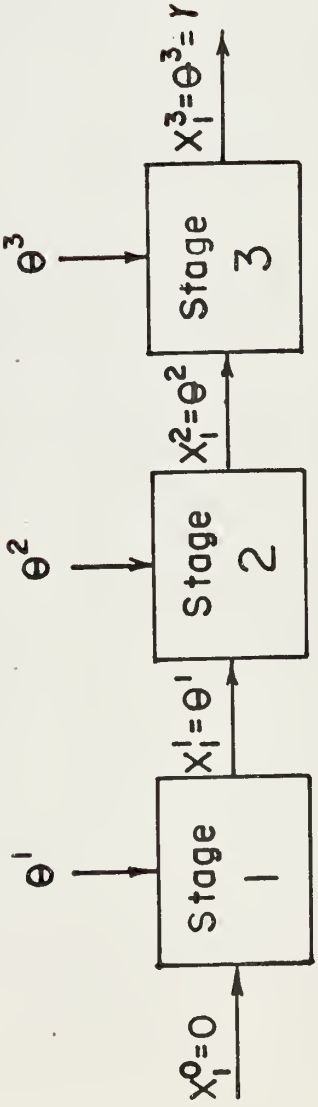


Fig. 2. Block diagram representation of the functional equations for the reactor system.

TABLE 1

PROGRAM SYMBOLS AND EXPLANATIONS

Symbol	Explanations	
DELX1	increment of x_1^1,	Δx_1^1
DELX2	increment of x_1^2,	Δx_1^2
DELT1	increment of θ^1,	$\Delta\theta^1$
DELT2	increment of θ^2,	$\Delta\theta^2$
FC	final conversion of reactant A,	γ
F1X12	minimum volume for one-stage process,	$f_1(x_1^2)$
F2X11	minimum volume for two-stage process,	$f_2(x_1^1)$
G1X10	volume of stage 1,	$g(x_1^0;\ \theta^1)$
G2X11	volume of stage 2,	$g(x_1^1;\ \theta^2)$
G3X12	volume of stage 3,	$g(x_1^2;\ \theta^3)$
SG2F1	sum of the volumes of stages 2 and 3,	$g(x_1^1;\ \theta^2) + f_1(x_1^2)$
TH1	conversion of reactant A at the outlet of stage 1,	θ^1
TH2	conversion of reactant A at the outlet of stage 2,	θ^2
X11	conversion of reactant A at the inlet of stage 2,	x_1^1
X12	conversion of reactant A at the inlet of stage 3,	x_1^2

TABLE 2A

OPTIMIZATION OF REACTOR VOLUME WITH TWO PHASE REACTION (COCURRENT)

```
   DIMENSION X12(21),X11(21),TH2(21),TH1(21),G3X12(21),F1X12(21)
   DIMENSION G2X11(21,21),SG2F1(21,21),F2X11(21),G1X10(21),SG1F2(21)
 1 FORMAT(9F8.3)
12 FORMAT(5F10.4)
   READ 1,FC,X12(1),X11(1),TH2(1),TH1(1),DELX2,DELX1,DELT2,DELT1
   CALC.G3X12(I)
   DO 11 I=2,21
   X12(I)=X12(I-1)+DELX2
   G3X12(I)=(FC-X12(I))/((1.-FC)*(1.-FC))
   F1X12(I)=G3X12(I)
   PUNCH 12,X12(I),G3X12(I),F1X12(I)
11 CONTINUE
   CALC.F2X11(J)
   DO 21 J=2,21
   X11(J)=X11(J-1)+DELX1
   DO 22 I=J,21
   TH2(I)=TH2(I-1)+DELT2
   G2X11(J,I)=(TH2(I)-X11(J))/(1.-TH2(I))/(1.-TH2(I))
   SG2F1(J,I)=G2X11(J,I)+F1X12(I)
   IF (I-J)23,23,24
23 F2X11(J)=SG2F1(J,I)
   PUNCH 12,X11(J),TH2(I),G2X11(J,I),F1X12(I),F2X11(J)
24 IF(F2X11(J)-SG2F1(J,I))22,22,25
25 F2X11(J)=SG2F1(J,I)
   PUNCH 12,X11(J),TH2(I),G2X11(J,I),F1X12(I),F2X11(J)
22 CONTINUE
21 CONTINUE
   CALC.F3X10
   DO 31 J=2,21
   TH1(J)=TH1(J-1)+DELT1
    G1X10(J)=TH1(J)/((1.-TH1(J))*(1.-TH1(J)))
   SG1F2(J)=G1X10(J)+F2X11(J)
   IF(J-2)32,32,33
32 F3X10=SG1F2(J)
   PUNCH 12,TH1(J),G1X10(J),F2X11(J),F3X10
33 IF(F3X10-SG1F2(J))31,31,34
34 F3X10=SG1F2(J)
   PUNCH 12,TH1(J),G1X10(J),F2X11(J),F3X10
31 CONTINUE
   END
```

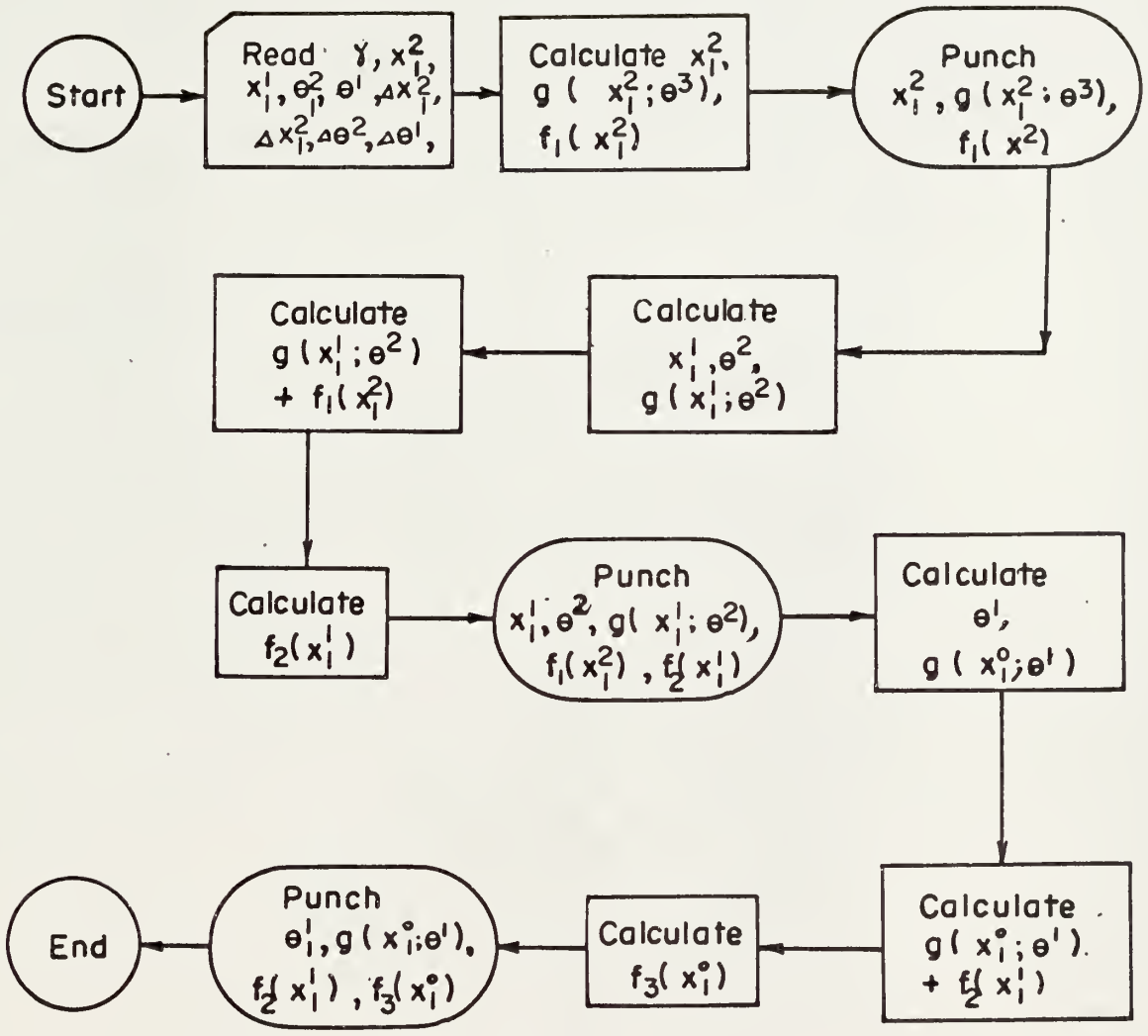


Fig.3. Computer flow diagram.

TABLE 3a

OPTIMAL TABLE (ONE STAGE COCURRENT PROCESS
WITH THE FINAL CONVERSION, $\gamma = 0.2$)

x_1^2	$g(x_1^2; \theta^3)$	$f_1(x_1^2)$	$x_1^3 = \theta^2$
0.00	0.3125	0.3125	0.200
0.01	0.2969	0.2969	0.200
0.02	0.2813	0.2813	0.200
0.03	0.2656	0.2656	0.200
0.04	0.2500	0.2500	0.200
0.05	0.2344	0.2344	0.200
0.06	0.2188	0.2188	0.200
0.07	0.2031	0.2031	0.200
0.08	0.1875	0.1875	0.200
0.09	0.1719	0.1719	0.200
0.10	0.1563	0.1563	0.200
0.11	0.1406	0.1406	0.200
0.12	0.1250	0.1250	0.200
0.13	0.1094	0.1094	0.200
0.14	0.0938	0.0938	0.200
0.15	0.0781	0.0781	0.200
0.16	0.0625	0.0625	0.200
0.17	0.0469	0.0469	0.200
0.18	0.0313	0.0313	0.200
0.19	0.0156	0.0156	0.200
0.20	0.0000	0.0000	0.200

TABLE 3b

OPTIMAL TABLE (TWO STAGE COCURRENT PROCESS WITH THE FINAL CONVERSION, $\gamma = 0.2$)

x_1^1	$x_1^2 = \theta^2$	$g(x_1^1; \theta^2)$	$f_1(x_1^2)$	$f_2(x_1^1)$
0.00	0.40	0.1389	0.1389	0.2778
0.01	0.11	0.1387	0.1236	0.2623
0.02	0.11	0.1233	0.1236	0.2469
0.03	0.12	0.1232	0.1087	0.2319
0.04	0.12	0.1082	0.1087	0.2169
0.05	0.13	0.1082	0.0941	0.2023
0.06	0.13	0.0936	0.0941	0.1876
0.07	0.14	0.0936	0.0798	0.1733
0.08	0.14	0.0793	0.0798	0.1591
0.09	0.15	0.0793	0.0658	0.1451
0.10	0.15	0.0654	0.0658	0.1311
0.11	0.16	0.0654	0.0521	0.1175
0.12	0.16	0.0518	0.0521	0.1038
0.13	0.17	0.0518	0.0387	0.0905
0.14	0.17	0.0385	0.0387	0.0771
0.15	0.18	0.0385	0.0255	0.0640
0.16	0.18	0.0254	0.0255	0.0509
0.17	0.19	0.0255	0.0126	0.0381
0.18	0.19	0.0126	0.0126	0.0252
0.19	0.20	0.0193	0.0000	0.0193
0.20	0.20	0.0000	0.0000	0.0000

TABLE 3c

OPTIMAL TABLE (THREE STAGE COCURRENT PROCESS WITH THE FINAL CONVERSION, $\gamma = 0.2$)

x_1^0	$x_1^1 = \theta^1$	$x_1^2 = \theta^2$	$x_1^3 = \theta^3$	$g(x_1^0; \theta^1)$	$g(x_1^1; \theta^2)$	$g(x_1^2; \theta^3)$	$f(x_1^0)$
0.00	0.07	0.14	0.20	0.0809	0.0946	0.0938	0.27

TABLE 4a

OPTIMAL TABLE (ONE STAGE COUNTERCURRENT PROCESS WITH THE FINAL CONVERSION, $\gamma = 0.2$)

x_1^2	$g(x_1^2;\ \theta^3)$	$f_1(x_1^2)$	$x_1^3 = \theta^3$
0.00	0.3125	0.3125	0.20
0.01	0.2932	0.2932	0.20
0.02	0.2744	0.2744	0.20
0.03	0.2560	0.2560	0.20
0.04	0.2381	0.2381	0.20
0.05	0.2206	0.2206	0.20
0.06	0.2035	0.2035	0.20
0.07	0.1868	0.1868	0.20
0.08	0.1705	0.1705	0.20
0.09	0.1545	0.1545	0.20
0.10	0.1389	0.1389	0.20
0.11	0.1236	0.1236	0.20
0.12	0.1087	0.1087	0.20
0.13	0.0941	0.0941	0.20
0.14	0.0798	0.0798	0.20
0.15	0.0658	0.0658	0.20
0.16	0.0521	0.0521	0.20
0.17	0.0387	0.0387	0.20
0.18	0.0255	0.0255	0.20
0.19	0.0126	0.0126	0.20
0.20	0.0000	0.0000	0.20

TABLE 4b

OPTIMAL TABLE (TWO STAGE COUNTERCURRENT PROCESS WITH THE FINAL CONVERSION, γ = 0.2)

x_1^1	$x_1^2 = \theta^2$	$g(x_1^1; \theta^1)$	$f_1(x_1^2)$	$f_2(x_1^1)$
0.00	0.10	0.1389	0.1389	0.2778
0.01	0.11	0.1387	0.1236	0.2623
0.02	0.11	0.1233	0.1236	0.2469
0.03	0.12	0.1232	0.1087	0.2319
0.04	0.12	0.1082	0.1087	0.2169
0.05	0.13	0.1082	0.0941	0.2023
0.06	0.13	0.0936	0.0941	0.1876
0.07	0.14	0.0936	0.0798	0.1733
0.08	0.14	0.0793	0.0798	0.1591
0.09	0.15	0.793	0.0658	0.1451
0.10	0.15	0.0654	0.0658	0.1311
0.11	0.16	0.0654	0.0521	0.1175
0.12	0.16	0.0518	0.0521	0.1038
0.13	0.17	0.0518	0.0387	0.0905
0.14	0.17	0.0385	0.0387	0.0771
0.15	0.18	0.0385	0.0255	0.0640
0.16	0.18	0.0254	0.0255	0.0509
0.17	0.19	0.0126	0.0255	0.0381
0.18	0.19	0.0126	0.0126	0.0252
0.19	0.20	0.0126	0.0000	0.0126
0.20	0.20	0.0000	0.0000	0.0000

TABLE 4c

OPTIMAL TABLE (THREE STAGE COUNTERCURRENT PROCESS WITH THE FINAL CONVERSION, $\gamma = 0.2$)

x_1^0	$x_1^1 = \theta^1$	$x_1^2 = \theta^2$	$x_1^3 = \theta^3$	$g(x_1^0; \theta^1)$	$g(x_1^1; \theta^2)$	$g(x_1^2; \theta^3)$	$f_3(x_1^0)$
0.00	0.06	0.13	0.20	0.0798	0.0936	0.0941	0.2674

TABLE 5

OPTIMAL REACTOR VOLUMES

(1) Cocurrent system

Conversion, %	Volume ft^3 V^1	V^2	V^3	Total
20	0.0865	0.0897	0.0931	0.2693
40	0.2427	0.2638	0.2833	0.7898
80	1.775	2.235	2.700	6.710
95	10.947	16.000	20.000	46.947

(2) Countercurrent system

Conversion, %	Volume ft^3 V^1	V^2	V^3	Total
20	0.0890	0.0894	0.0890	0.2674
40	0.2535	0.2538	0.2535	0.7607
80	1.610	1.590	1.610	9.810
95	6.076	6.043	6.076	18.195
99	20.482	20.062	20.482	61.026

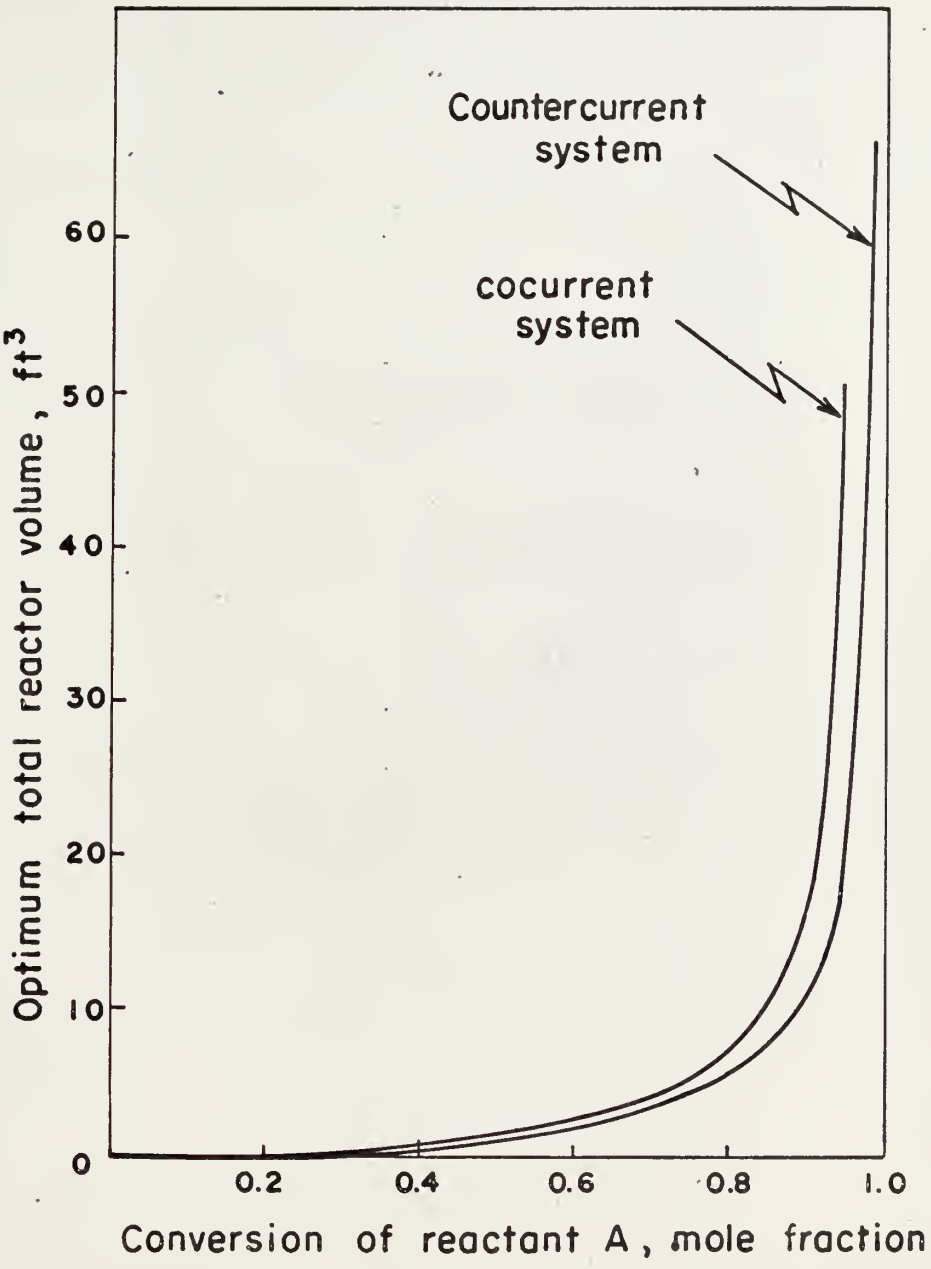


Fig. 4. Optimal total reactor volume vs conversion for two continuous flow stirred tank reactor systems.

reaction scheme because the former requires less reactor volume to achieve the same degree of conversion. As seen in Fig. 5, a considerable difference in the optimal total reactor volumes between the two systems occurs, especially at high conversions.

(3) In the cocurrent flow reaction scheme, the volume ratios of stages 2 and 3 to stage 1 are comparable with those given in Ref. 2 for the case of a second order irreversible reaction. For comparison, the numerical values are listed in Table 6. It can be seen that the differences become greater as the conversion increases because a slight increase in conversion requires a large increase in reactor volume at a higher conversion. Since finite numbers of grid points are chosen for computation, considerable interpolation is required, especially at higher conversions. The optimal volume ratios vs. conversion of reactant A for both cases are plotted in Fig. 6.

A comparison of the optimal and non-optimal values for four cases are given in Table 7.

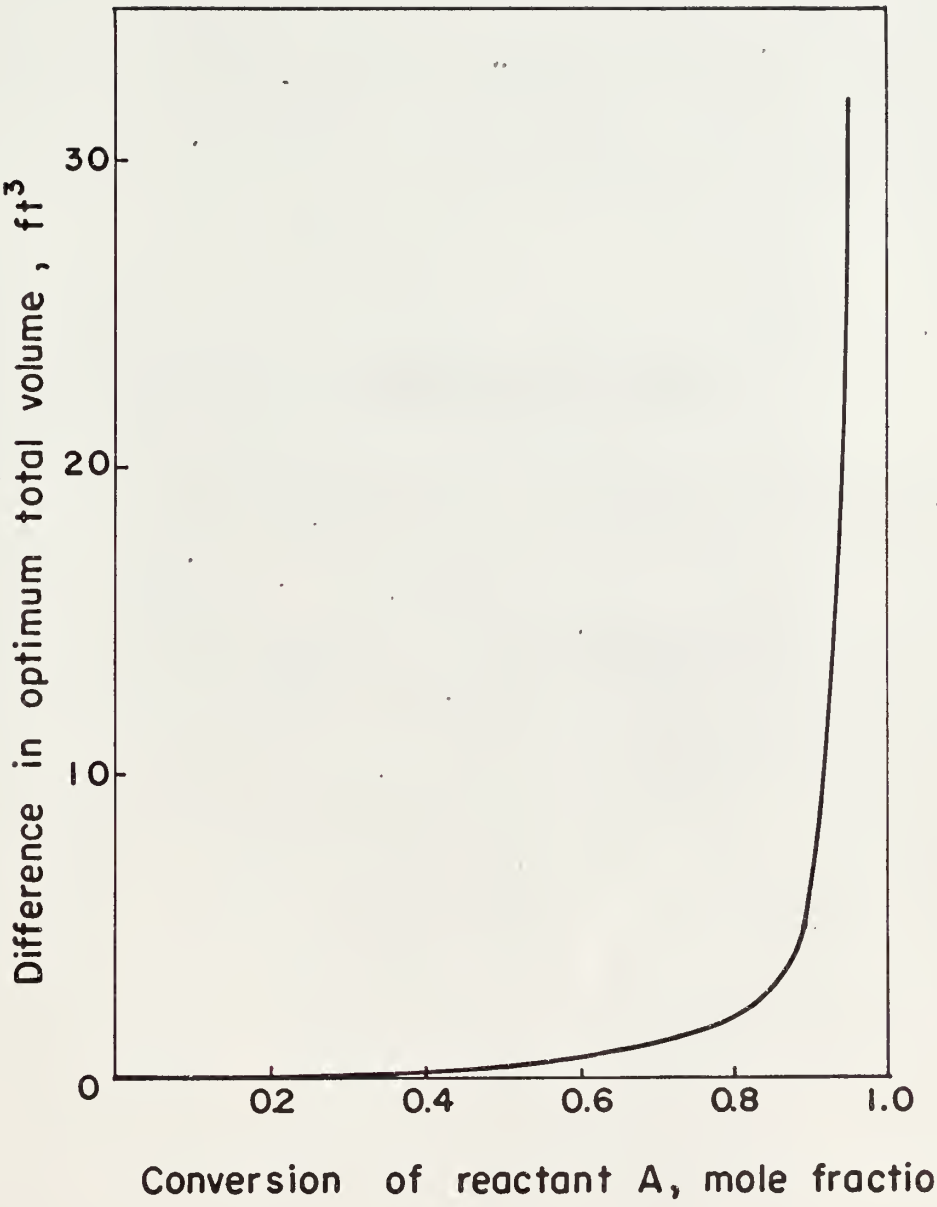


Fig. 5. Difference in the optimum total volume between the cocurrent and countercurrent systems.

TABLE 6

RATIOS OF INDIVIDUAL OPTIMAL REACTOR VOLUMES FOR THE COCURRENT SYSTEM

Conversion, %	V_2/V_1 This Study	Ref [2]*
20	1.037	1.037
40	1.087	1.085
80	1.259	1.256
95	1.462	1.450

Conversion, %	V_3/V_1 This Study	Ref [2]*
20	1.076	0.175
40	1.167	1.170
80	1.520	1.523
95	1.852	1.956

*Obtained by interpolation of the results of the Lagrangian multiplier solution given in Ref. [2].

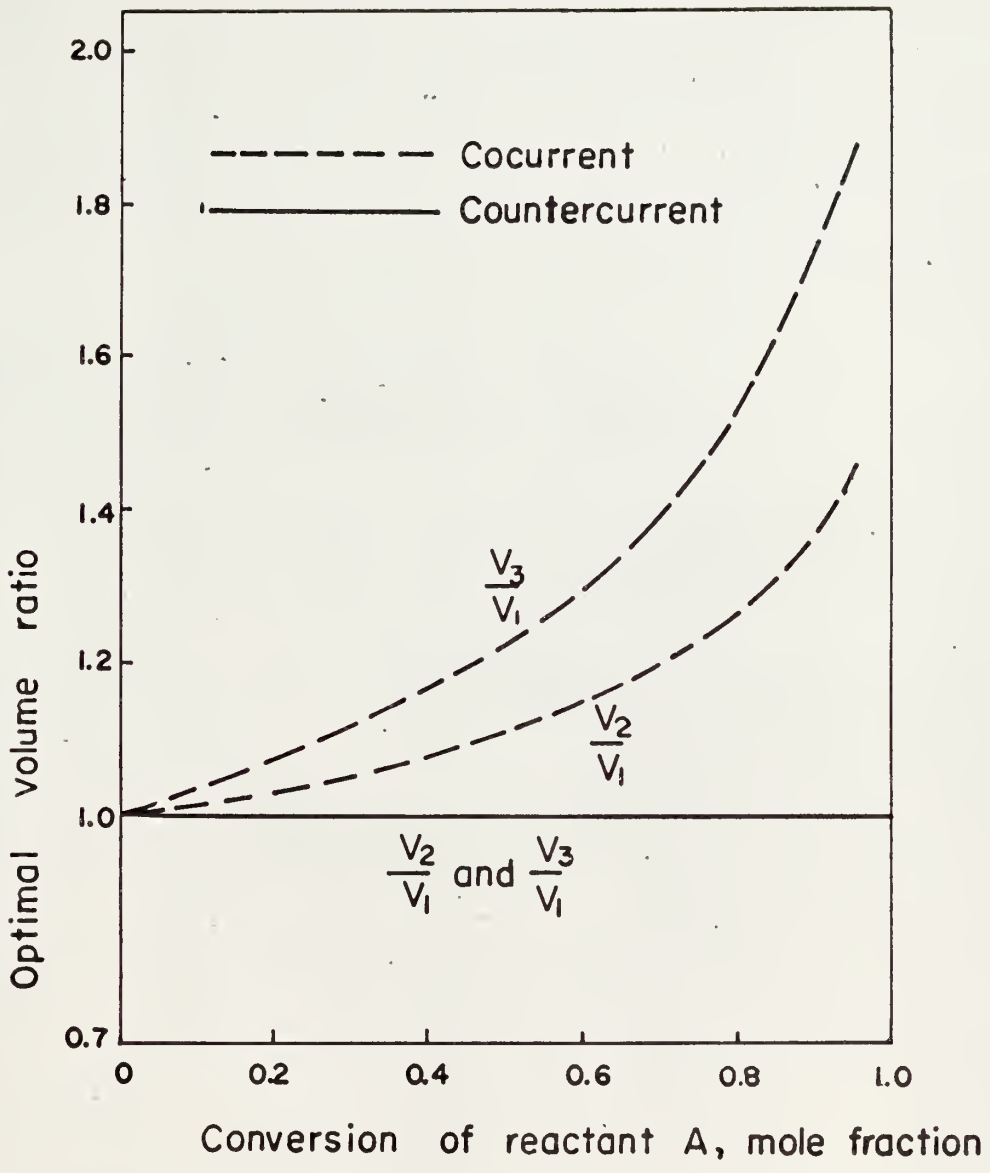


Fig. 6. Optimal ratio of individual reactor volume.

TABLE 7

COMPARISON OF OPTIMAL AND NON-OPTIMAL VALUES

(1) Cocurrent System

Conversion, %	Case	$x_1^1 = \theta^1$	$x_1^2 = \theta^2$	V^1 ft^3	V^2 ft^3	V^3 ft^3	Total ft^3
40	Optimal	0.168	0.298	0.2471	0.2638	0.2833	0.7898
	Non-optimal	0.162	0.294	0.2307	0.2539	0.3056	0.7902
95	Optimal	0.740	0.900	10.947	16.000	20.000	46.947
	Non-optimal	0.730	0.890	10.014	13.223	24.000	47.237

(2) Countercurrent System

Conversion, %	Case	$x_1^1 = \theta^1$	$x_1^2 = \theta^2$	V^1 ft^3	V^2 ft^3	V^3 ft^3	Total ft^3
40	Optimal	0.132	0.268	0.2535	0.2538	0.2535	0.7607
	Non-optimal	0.124	0.276	0.2359	0.2900	0.2359	0.7618
95	Optimal	0.233	0.717	6.076	6.043	6.076	18.195
	Non-optimal	0.224	0.726	5.773	6.688	5.773	18.233

References:

1. Bellman, R., "Dynamic Programming," Princeton Univ. Press, New Jersey, 1957.

2. Fan, L. T. and C. S. Wang, "The Discrete Maximum Principle," John Wiley & Sons, New York, 1964.

3. Aris, R., "Dynamic Programming," Socony Mobil Oil Company, Dallas, Texas, 1963.

4. Tou, J. T., "Modern Control Theory," McGraw Hill, New York, 1964.

5. Aris, R., "Discrete Dynamic Programming," Blaisdell, New York, 1959.

6. Bellman, R. and Dreyfus, S., "Applied Dynamic Programming," Princeton Univ. Press, New Jersey, 1962.

7. Lee, E. S., Unpublished report.

NOMENCLATURE

b_i : Numbers of hours required to produce a ton of grade i, $\frac{hr}{ton}$.

c : Total production hours, hr.

N_A : Number of mbles of reactant A, 16-mole .

P_i : Net profit per ton of grade i, $\frac{\$}{ton}$.

$-r_A$: Reaction rate based on reactant A, $\frac{16\text{-mole}}{ft.^3\ sec}$.

V_i : Reactor volume, ft^3 .

x_1^n : Conversion of reactant A at the exit of stage n .

x_i : Number of tons of grade i produced in a week, $\frac{ton}{week}$.

S = P : Maximum return or net profit, $\frac{\$}{week}$.

Greek Letters

θ^n : Conversion of reactant A at the inlet of stage n .

γ : Final conversion of reactant A .

CHAPTER III

OPTIMIZATION OF A MULTIEFFECT MULTISTAGE EVAPORATION SYSTEM BY DYNAMIC PROGRAMMING

The optimization of a multieffect multistage evaporator system with a nominal capacity of 50 MM gallons per day is considered here [1, 2].

There are 23 stages each in the first effect and second effect, and 22 stages in the third effect. The production of distillate in each stage is achieved by adiabatic flash vaporization such that the temperature of the flashing brine decreases as it cascades down stage by stage. A portion of the flashing brine from each effect is recycled back through the condenser tubes on which water vapor is condensing, so that the make-up feed and the recycle brine are preheated prior to mixing. The make-up feed together with the recycle brine in the first effect is finally heated to the maximum flashing temperature by a shell and tube brine heater with low pressure steam from an adjacent power plant. The diagram of the process is shown in Fig. 1.

The maximum brine temperature is limited by scale formation and the lower temperature end is slightly higher than the temperature of the make-up feed because a certain temperature difference for heat transfer must be maintained for heating the make-up and recycle brine.

This scheme is more efficient thermodynamically than recycling the blowdown from the last effect directly to the first effect, because the mixing streams are at the same temperature and the concentration differences between the mixing streams are reduced as the whole system is divided into three effects. The free energy decrease due to mixing, the thermodynamic irreversibility, is thus reduced.

Furthermore, the heat recovery becomes more efficient as the number of

Fig. 1. Process flow diagram of the multistage multieffect flash evaporation system.

stages used for flashing and preheating increases; inter-effect recycling makes it possible to add more stages per temperature gradient. Theoretically, the larger the number of stages, the higher the performance ratio (ratio of distillate production to steam consumption), but the number of stages cannot be increased without limit because a certain pressure gradient should be maintained for the flow of the flashing brine.

The optimization involves the following factors:

(1) number of total stages

(2) total temperature differences (temperature differences between the flashing and recycle brine)

(3) number of stages allocated to each effect

(4) exit temperature and concentration of each effect

(5) allocation of distillate production in each effect

(6) brine velocities of various concentrations which affect the overall heat transfer coefficients of heater and condenser tubes.

We shall, however, take only the role of the total temperature differences and exit brine temperatures of each effect into account.

In this problem, the temperatures of the flashing brine is chosen as the state variable and the recycle ratio of each effect as the decision variable. The ratio of energy input to the make-up feed, q/F, is taken as the parameter. For clarity, performance and cost equations of this process are listed in Table 1 (see Appendices I and II for derivation).

1. STATEMENT OF PROBLEM

We shall employ dynamic programming to perform the optimization. The following conditions and assumptions are made in formulating this

optimization problem:

(1) Equal distillate production for each effect.

(2) Equal temperature drops of the flashing brine in each stage of the heat recovery section of each effect.

(3) Equal boiling point elevations for each stage such that the temperature profiles of the flashing brine and distillate are parallel.

(4) The temperature difference between the flashing and recycle brine is constant for the heat recovery section of each effect.

From the performance and cost equations given in Table 1, the following items and relations which are necessary for developing the functional relationships of dynamic programming are obtained.

(1) The steam cost is $\frac{2C_1 q}{F\lambda_s}$

(2) The fixed charge cost for the brine heater (see equation (3)) is

$$\frac{1.92\ C_2(1+\theta^1)}{U_B}\left\{\ln\left(24.4 + \frac{q}{0.96\ F(1+\theta^1)}\right) - \ln(24.4)\right\}$$

where θ^1 is the recycle ratio of the first effect which is related to the maximum brine and first blowdown temperatures x_1^0 and x_1^1 as given in equation (1) by taking material and energy balances for the first effect.

$$\theta^1 = \frac{1065 + 4.986x_1^1 - 5.594x_1^0}{5.748(x_1^0 - x_1^1)}$$

(3) The fixed charge cost for the condenser tubes in the heat recovery section of the first effect is

TABLE 1

SYSTEM EQUATIONS

The first stage

(1) Transformation equation

(material and energy balance)

$$x_1^1 = \frac{(5.748\theta^1 + 5.594)x_1^0 - 1065}{5.748\theta^1 + 4.986} \qquad (1)$$

(2) Steam cost

$$\frac{2C_1 q}{F\lambda_s} \qquad (2)$$

C_1 : given

λ_s : given

q/F : assumed

(3) Fixed charge cost for the brine heater

$$\frac{1.92C_2(1+\theta^1)}{U_B}\left\{\ln\left(24.4 + \frac{q}{0.96F(1+\theta^1)}\right) - \ln(24.4)\right\} \qquad (3)$$

C_2 : given

U_B : given

(4) Fixed charge cost for the condenser tubes, heat recovery section

$$\frac{76.8C_3(1+\theta^1)\left\{0.96(1+\theta^1)(1065-0.608x_1^0) - \frac{q}{F}(5.748\theta^1 + 4.986)\right\}}{(U_1)_{av}\left\{\frac{41q}{F}(5.748\theta^1+4.986) - 0.96(1+\theta^1)(1463.9-0.608x_1^0+459.8\theta^1)\right\}} \qquad (4)$$

C_3 : given

$(U_1)_{av}$: given

TABLE 1 (Cont'd)

(5) Fixed charge cost for the condenser tubes, heat rejection section

$$\frac{12C_3}{(U_1)_{av}\left\{\frac{3}{0.952(1+\theta^2)} + \frac{2}{0.96(1+\theta^1)} - \frac{12F}{q}\right\}} \qquad (5)$$

(6) Recycle cost

$$\frac{288C_4 \times \theta^1(P_0 - P_1)}{62.5 \times 550 \times 3600 \times 4.85} \qquad (6)$$

C_4 : given

P_0 : from steam table

P_1 $\exp\left\{14.07 - \frac{9 \times 3600}{5(x_1 - 32) + 1989}\right\}$

The second stage

(1) Transformation equation (material and energy balance)

$$x_1^2 = \frac{(5.685\theta^2 + 4.594)x_1^1 - 1065}{5.685\theta^2 + 3.986} \qquad (7)$$

(2) Fixed charge cost for the condenser tubes, heat recovery section

$$\frac{76.16C_3(1+\theta^2)\left\{0.952(1+\theta^2)(1065 - 0.608x_1^1) - \frac{q}{F}(5.685\theta^2 + 3.986)\right\}}{(U_2)_{av}\left\{\frac{41q}{F}(5.685\theta^2 + 3.986) - 0.952(1+\theta^2)(1383.9 - 0.608x_1^1 + 454.8\theta^2)\right\}} \qquad (8)$$

$(U_2)_{av}$ + given

TABLE 1 (Cont'd)

(4) Recycle cost

$$\frac{288C_4\,\theta^2(P_1 - P_2)}{62.5 \times 550 \times 3600 \times 0.85} \tag{10}$$

$$P_2 = \exp\left\{14.07 - \frac{9 \times 3600}{5(x_1^2-32) + 1989}\right\}$$

The third stage

(1) Transformation equation (material and energy balance)

$$x_1^3 = \frac{(5.58\theta^3 + 3.594)x_1^2 - 1065}{5.58\theta^3 + 2.986} \tag{11}$$

(2) Fixed charge cost for the condenser tubes, heat recovery section

$$\frac{75.2C_3(1+\theta^3)\left\{0.94(1+\theta^3)(1065 - 0.608x_1^2) - \frac{q}{F}(5.58\theta^3 + 2.986)\right\}}{(U_3)_{av}\left\{\frac{41q}{F}(5.58\theta^3+2.986)-0.94(1+\theta^3)(1303.9-0.609x_1^2+446.4\theta^3)\right\}} \tag{12}$$

$$(U_3)_{av} : \text{given}$$

(3) Fixed charge cost for the condenser tubes, heat rejection section

$$\frac{7.52C_3(1+\theta^3)(5.58\theta^3 + 2.986)}{(U_3)_{av}\left\{15.58\theta^3+2.986)+\left\{\frac{2F}{q}(5.58\theta^3+3.594)x_1^2-1065\right\}0.94(1+\theta^3)- \frac{0.94F}{q}(1+\theta^3)(2T_F+8)(5.58\theta^3+2.986)\right\}} \tag{13}$$

(4) Recycle cost

$$\frac{288C_4\,\theta^3(P_2 - P_3)}{62.5 \times 550 \times 3600 \times 0.85}$$

TABLE 1 (Cont'd)

$$P_3 = \exp\left\{14.07 - \frac{9 \times 3600}{5(x_3-32) + 1989}\right\}$$

Others

(1) Dumping cost for the distillate and blowdown	$\frac{288C_4(14.7 - P_3)}{62.5 \times 550 \times 3600 \times 0.85}$	(15)
(2) Pumping cost for the make-up feed	$\frac{2.36C_4(\Delta H_0 + 50)}{550 \times 3600}$	(16)
	$\Delta H_0 = \frac{144(P_0 - 14.7)}{62.5}$	
(3) Structure cost	$\frac{43.2 \times 7.48 \times 24}{62.4 \times 5 \times 10^7}$	(17)

$$\frac{76.8C_3(1+\theta^1)\left\{0.96(1+\theta^1)(1065-0.608x_1^1)-\frac{q}{F}(5.748\theta^1+5.594)\right\}}{(U_1)_{av}\left\{\frac{41q}{F}(5.748\theta^1+5.594)-0.96(1+\theta^1)(1512.5-0.608x_1^1+459.8\theta^1)\right\}}$$

It should be noted that x_1^0 is eliminated so that the fixed charge cost is expressed as a function of x_1^1 and θ^1 .

(4) The fixed charge cost for the condenser tubes in the heat recovery section of the second effect is

$$\frac{76.16C_3(1+\theta^2)\left\{0.952(1+\theta^2)(1065-0.608x_1^2)-\frac{q}{F}(5.685\theta^2+4.594)\right\}}{(U_2)_{av}\left\{\frac{41q}{F}(5.685\theta^2+4.594)-0.952(1+\theta^2)(1432.5-0.608x_1^2+454.8\theta^2)\right\}}$$

where θ^2 is the recycle ratio of the second effect. The recycle ratio is related to the first and second blowdown temperatures x_1^1 and x_1^2 as given in equation (7) of Table 1. Equation (7), which is obtained from the material and energy balances around the second effect, is

$$\theta^2 = \frac{1065 + 3.986x_1^2 - 4.594x_1^1}{5.685(x_1^1 - x_1^2)}$$

(5) The fixed charge cost for the condenser tubes in the heat recovery section of the third effect is

$$\frac{75.2C_3(1+\theta^3)\left\{0.94(1+\theta^3)(1065-0.608x_1^3)-\frac{q}{F}(5.58\theta^3+3.594)\right\}}{(U_3)_{av}\left\{\frac{41q}{F}(5.58\theta^3+3.594)-0.94(1+\theta^3)(1452.5-0.608x_1^3+446.4\theta^3)\right\}}$$

where θ^3 is the recycle ratio of the third effect, which is related to the second and final blowdown temperatures x_1^2 and x_1^3 as given in equation (11). By taking material and energy balances around the third effect, equation (11) is obtained as

$$\theta^3 = \frac{1065 + 2.986x_1^3 - 3.594x_1^2}{5.58(x_1^2 - x_1^3)}$$

(6) The fixed charge cost for the condenser tubes in the heat rejection section of the third effect is

$$\frac{7.52C_3(1+\theta^3)}{(U_3)_{av}\left\{1 + \frac{1.88F}{q}(1+\theta^3)x_1^3 - \frac{1.88F}{q}(1+\theta^3)(T_F+4)\right\}}$$

With these cost functions in hand, we can write the unit production cost for each stage, which, in the language of dynamic programming, is the so-called return function as

$$G^1(x_1^1;\theta^1) = \text{eq. (2)} + \text{eq. (3)} + \text{eq. (4)}$$

$$G^2(x_1^2;\theta^2) = \text{eq. (8)}$$

$$G^3(x_1^3;\theta^3) = \text{eq. (12)} + \text{eq. (13)}$$

The fixed charge costs for the condenser tubes in the heat rejection sections of the first and second effects and the recycle costs for each effect are not included in the optimization because

(1) the determination of the optimal tube area for the heat rejection section involves decisions in memory.

(2) the total recycle cost is not only approximately constant but is of minor significance to the total production cost (see Appendix II).

Therefore the cost items in Table I which are excluded from the present consideration will be added to the optimal production cost after the optimization has been carried out.

Now, let us consider the problem in more detail so that it will enable

us to choose the computational ranges of variables.

First of all, we may observe that in computing $G^1(x_1^1;\theta^1)$, the steam cost is constant for a given q/F and the fixed charge cost for the brine heater is nearly proportional to θ^1. Furthermore, from the relation of the energy input to the brine heater,

$$q/F = (1+\theta^1)(C_p)_{av}\Delta t_1 .$$

With a given q/F, the larger the value θ^1 is, the smaller the temperature rise through the heater Δt_1, and the larger the fixed charge cost for the condenser tubes. It is obvious that Δt_1 directly affects the average temperature difference for heat transfer of the condenser tubes in the heat recovery section of the first effect.

In the derivation in Appendix II, we have shown that the condenser tube areas are approximately equal to

$$A_n = \frac{q_n}{(U_n)_{av}\Delta t_n} = \frac{\frac{F}{6}(\lambda_n)_{av}}{(U_n)_{av}\Delta t_n} \qquad n = 1, 2, 3$$

and we also have the formula

$$\frac{q}{F} = (1 + r_n)(C_p)_{av}\Delta t_n . \qquad n = 1, 2, 3$$

where r_n is replaced by θ^n in this formulation.

For a given q/F, $\frac{1}{\Delta t_n}$ is an approximately linear function of θ^n and so is A_n. With q/F fixed, $G^1(x_1^1;\theta^1)$ is approximately a linear function of θ^1 since the fixed charge cost for the condenser tubes takes on the major part of the variable cost in $G^1(x_1^1;\theta^1)$. It is also true of $G^2(x_1^2;\theta^2)$ and $G^3(x_1^3;\theta^3)$ because they contain only the fixed charge cost for the condenser

tubes.

From the above considerations, it is intuitively seen that the smaller the θ^n's, the smaller the unit production cost.

If we consider the limiting case where θ^n goes to zero, the process turns out to be unfeasible.

Actually, from the material and energy balance

$$\frac{F}{2} \times (\lambda)_{av} = F(1+\theta)(C_p)_{av}(x_1^0 - x_1^3)$$

for a one stage process, we see that the magnitude of θ is approximately 2.36 as follows

$$\frac{F}{2} (1000) = F(1+\theta)(0.96)(250-95)$$

$$\theta \doteq 2.36 .$$

For a three stage process, this is still true because $\frac{F}{2}$ becomes $\frac{F}{6}$, and $x_1^0 - x_1^3$ becomes approximately $\frac{1}{3}(x_1^0-x_1^3)$ and thus the magnitudes of θ^n remain approximately 2.36. It does not mean that θ^n must always take on this value, one of the θ^n can take on a value much smaller than 2.36, but the other two θ^n will become larger at the expense of its reduction.

Since

$$q_1 \doteq F(1+\theta^1)(C_p)_{f1}(x_1^0-x_1^1) = \frac{F}{6} (\lambda_1)_{av} .$$

$$q_2 \doteq F(1+\theta^2)(C_p)_{f2}(x_1^1-x_1^2) = \frac{F}{6} (\lambda_2)_{av} .$$

$$q_3 \doteq F(1+\theta^3)(C_p)_{f3}(x_1^2-x_1^3) = \frac{F}{6} (\lambda_3)_{av} .$$

and

$$(\lambda_1)_{av} < (\lambda_2)_{av} < (\lambda_3)_{av} .$$

we can see that

$$q_1 < q_2 < q_3$$

and hence

$$x_1^0 - x_1^1 < x_1^1 - x_1^2 < x_1^2 - x_1^3$$

for approximately equal θ^n, n = 1, 2, 3. This observation suggests the choices

$$x_1^0 - x_1^1 < \frac{1}{3}(x_1^0 - x_1^3) ,$$

$$x_1^1 - x_1^2 \doteq \frac{1}{3}(x_1^0 - x_1^3) ,$$

$$x_1^2 - x_1^3 > \frac{1}{3}(x_1^0 - x_1^3) .$$

According to the dynamic programming algorithm [Ref. 3], the functional equations are written as:

(1) For a one-stage process including only the first stage (see Fig. 2)

$$f_1(x_1^1) = \min_{\theta^1} \left\{ G^1(x_1^1;\theta^1) \right\}$$

(2) For a two-stage process including the first and second stages (see Fig. 2)

$$f_2(x_1^2) = \min_{\theta^2} \; G^2(x_1^2;\theta^2) + f_1(x_1^1)$$

(3) For a three stage process including all the stages (see Fig. 2)

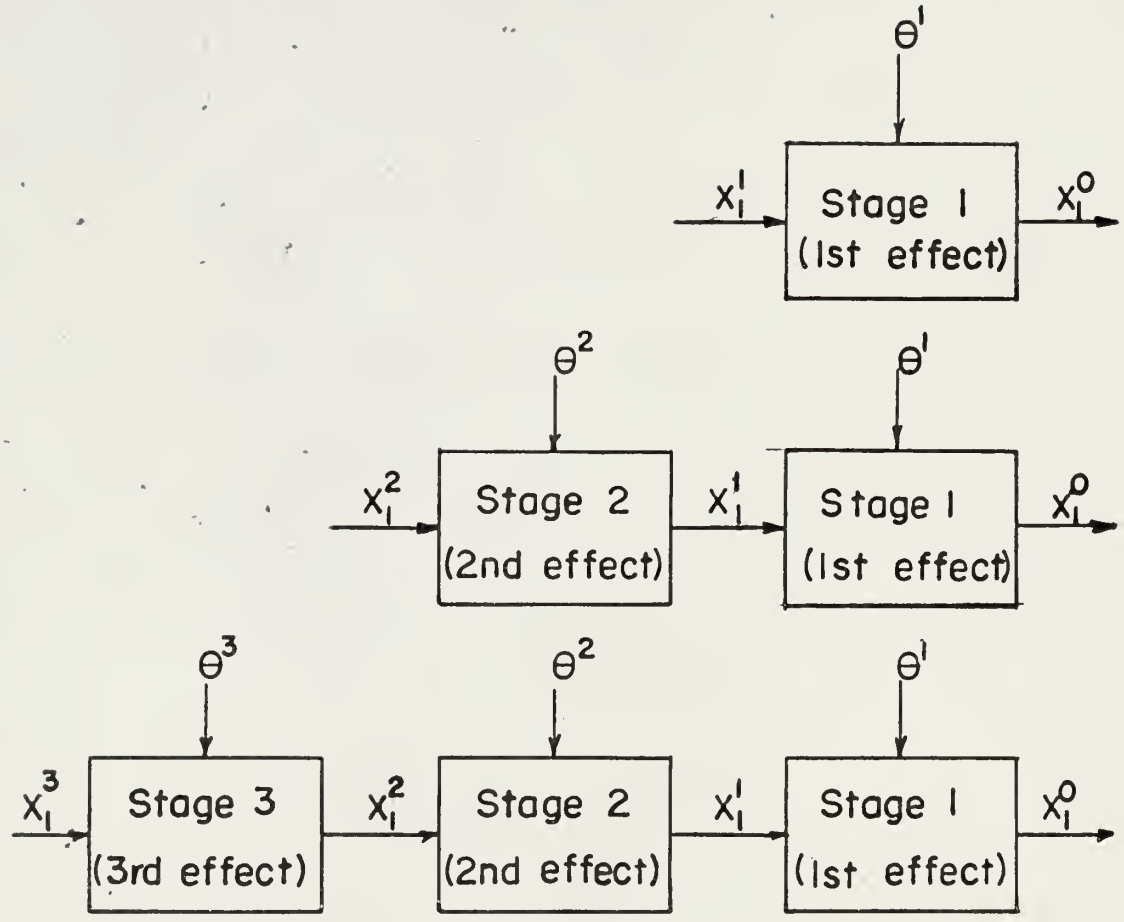


Fig. 2. Schematic diagram showing the numbering of stages used for the imbedding scheme.

$$f_3(x_1^3) = \min_{\theta^3} \; G^3(x_1^3;\theta^3) + f_2(x_1^2) \; .$$

2. COMPUTATIONAL SCHEME

The computational procedure is summarized below:

(A) Computation of $f_1(x_1^1)$

(1) Choose $x_1^0 = 250$, $\quad q/F = 26.7$

(2) Choose ten grid points for x_1^1 with increment 0.3

$$x_1^1 = 201.7 \sim 204.4$$

(3) Computate for each path

$$G^1(x_1^1;\theta^1)$$

(4) Set $f_1(x_1^1)$ equal to $G^1(x_1^1;\theta^1)$ corresponding to each x_1^1 .

(B) Computation of $f_2(x_1^2)$

(1) Choose $x_1^2 = 148.8$, $\quad q/F = 26.7$

(2) Compute $G^2(x_1^2;\theta^2)$ for each path connecting

$$x_1^2 = 148.8 \quad \text{to} \quad x_1^1 = 201.7 \sim 204.4 \; .$$

(3) Add the previously calculated $f_1(x_1^1)$ to $G^2(x_1^1;\theta^2)$ and find

$$f_2(x_1^2)$$

(4) Compute $f_2(x_1^2)$ by varying x_1^2 with increment 0.3 for the range

$$148.8 \leq x_1^2 \leq 151.5 \; .$$

(C) Computation of $f_3(x_1^3)$

(1) Choose $x_1^3 = 90$, $q/F = 26.7$

(2) Compute $G^3(x_1^3;\theta^3)$ for each path connecting $x_1^3 = 90$ to $x_1^2 = 148.8 \sim 151.5$.

(3) Add the previously calculated $f_2(x_1^2)$ to $G^3(x_1^3;\theta^3)$ and find $f_3(x_1^3)$

(4) Compute $f_3(x_1^3)$ by varying x_1^3 with increment 0.5 for the range

$$90 \leqq x_1^3 \leqq 94.5 .$$

Repeat this computational procedure by varying q/F with increment 0.3 for $26.7 \leqq q/F \leqq 27.9$. The computational paths are shown in Fig. 3. The computer flow diagram is shown in Fig. 4 and the computer symbols and program are given in Tables 2a and 2b.

3. RESULTS AND DISCUSSION

The computations were carried out on an IBM 1620 computer, and the optimal tables are shown in Tables 3, 4 and 5. It is noted that for each q/F, the production cost becomes lower and lower as the final blowdown temperature x_1^3 goes down.

From the temperature profiles for the heat rejection section of the third effect, it is seen that (Fig. 5)

$$\frac{\Delta t_{3r} + \Delta t_{3j}}{2} \geqslant \frac{\Delta t_{3r}}{2} + 2$$

or $$\Delta t_{3j} \geqslant 4$$

where Δt_{3r} = temperature drop of the flashing brine across the heat

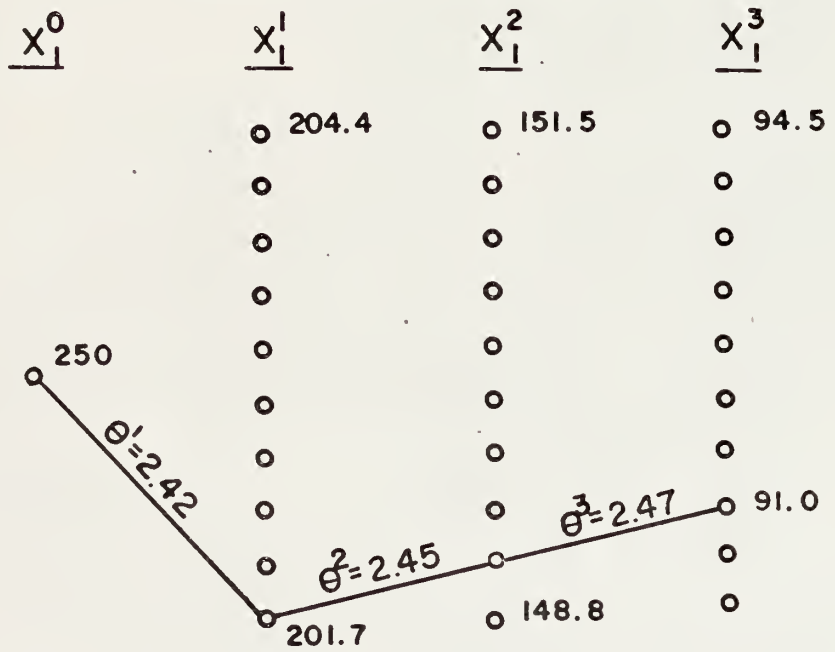


Fig. 3. Grid points of the state variable taken for computation. The connected line is the optimal path. (q/F = 27.0)

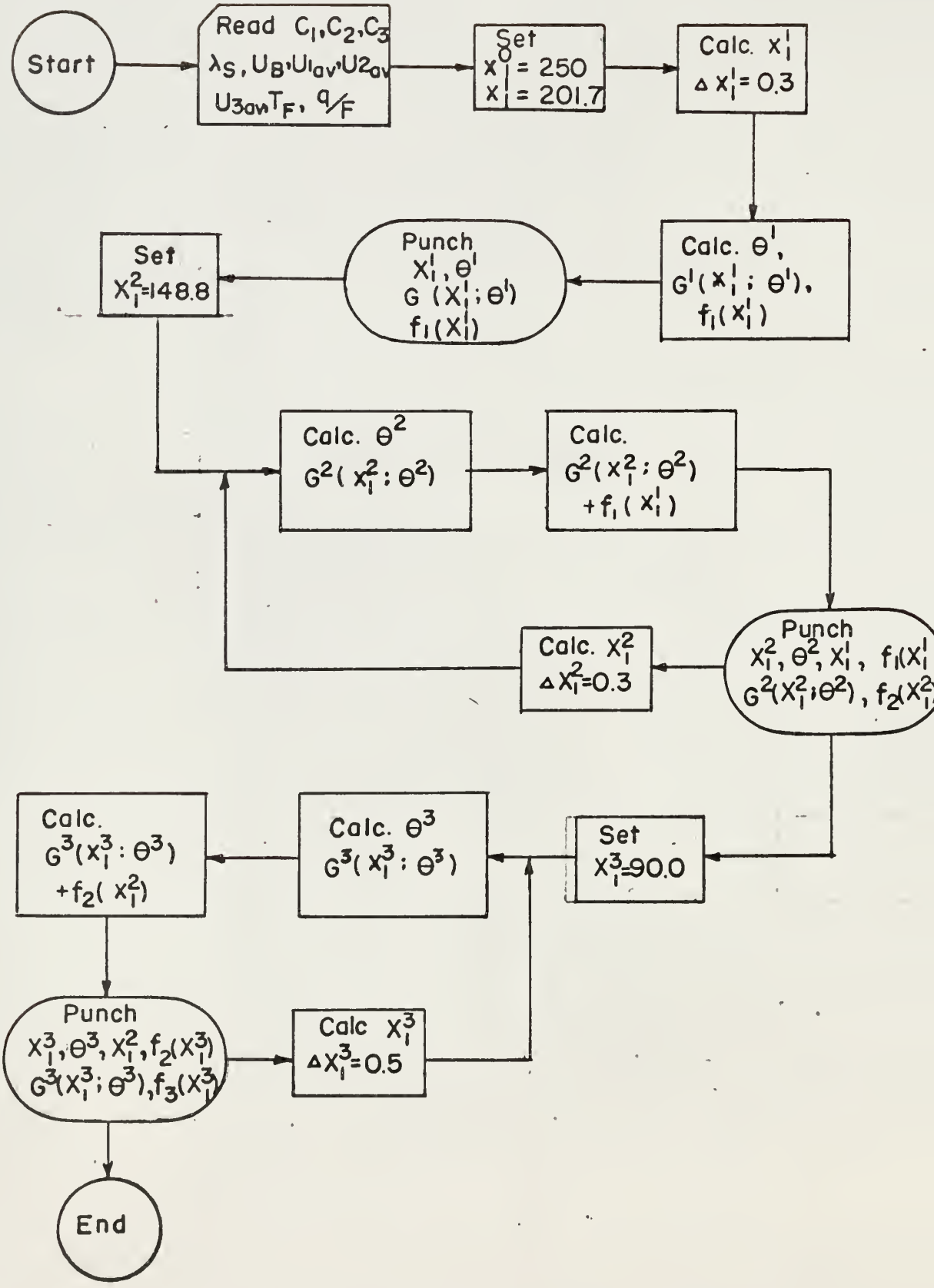


Fig. 4. Computer flow diagram.

TABLE 2a

EXPLANATION OF COMPUTER PROGRAM SYMBOLS

Symbol	Explanation
C1	unit steam cost, C_1
C2	unit fixed charge cost, brine heater, C_2
C3	unit fixed charge cost, condenser tubes, C_3
F1X1	maximum return function, one-stage process, $f_1(x_1^1)$
F2X2	maximum return function, two-stage process, $f_2(x_1^2)$
F3X3	maximum return function, three-stage process, $f_3(x_1^3)$
G1X1	return function, stage 1, $G^1(x_1^1;\theta^1)$
G2X2	return function, stage 2, $G^2(x_1^2;\theta^2)$
G3X3	return function, stage 3, $G^3(x_1^3;\theta^3)$
QDF	ratio of the energy input to the make-up feed, q/F
RMS	latent heat of the live steam, λ_s
SG12	sum of the return function of stage 2 and the maximum return function of the one-stage system, $G^2(x_1^2;\theta^2) + f_1(x_1^1)$
SG23	sum of the return function of stage 3 and the maximum return function of the two-stage system, $G^3(x_1^3;\theta^3) + f_2(x_1^2)$
TF	temperature of the make-up feed, T_F
TH1	ratio of the recycle brine in the first stage to the make-up feed, θ^1
TH2	ratio of the recycle brine in the second stage to the make-up feed, θ^2

TABLE 2a (Cont'd)

Symbol	Explanation
TH3	ratio of the recycle brine in the third stage to the make-up feed, θ^3
UB	overall heat transfer coefficient of the heater tubes, U_B
U1AV	average overall heat transfer coefficient of the condenser tubes, the first stage, $(U_1)_{av}$
U2AV	average overall heat transfer coefficient of the condenser tubes, the second stage, $(U_2)_{av}$
U3AV	average overall heat transfer coefficient of the condenser tubes, the third stage, $(U_3)_{av}$
X1	blowdown temperature, the first stage, x_1
X2	blowdown temperature, the second stage, x_2
X3	blowdown temperature, the third stage, x_3

TABLE 2B

OPTIMIZATION OF THE MULTIFLASH EVAPORATION PROCESS

```
      DIMENSION X1(11),X2(11),X3(11),G1X1(11),F1X1(11),TH1(11)
      DIMENSION F2X2(11),F3X3(11),TH2(11,11),TH3(11,11),G2X2(11,11)
      DIMENSION G3X3(11,11),SG12(11,11),SG23(11,11)
    1 FORMAT(6X,6E10.4)
   12 FORMAT(1H 2F10.2,2X,2E12.6)
   13 FORMAT(1H 3F10.2,F11.5,2F12.6)
      READ 1,C1,C2,C3,RMS,UB,U1AV
      READ 1,U2AV,U3AV,TF,QDF
      PRINT 1,C1,C2,C3,RMS,UB,U1AV
      PRINT 1,U2AV,U3AV,TF,QDF
      CALC.TH1(J),G1X1(J)
      X0=250.
      X1(1)=201.4
      DO 11 J=2,11
      X1(J)=X1(J-1)+.3
      TH1(J)=(1065.+4.986*X1(J)-5.594*X0)/(5.748*(X0-X1(J)))
      G1X1(J)=2.*C1*QDF/RMS+1.92*C2*(1.+TH1(J))*(LOG(24.4+QDF/(.96*(1.+
     1TH1(J))))-LOG(24.4))/UB+76.8*C3*(1.+TH1(J))*(.96*(1.+TH1(J))*(1065
     2.-.608*X1(J))-QDF*(5.748*TH1(J)+5.594))/U1AV/(41.*QDF*(5.748*TH1(J
     3)+5.594)-.96*(1.+TH1(J))*(1512.5-.608*X1(J)+459.8*TH1(J)))
      F1X1(J)=G1X1(J)
      PUNCH 12,X1(J),TH1(J),G1X1(J),F1X1(J)
   11 CONTINUE
      CALC.TH2(K,J),F2X2(K)
      X2(1)=148.5
      DO 21 K=2,11
      X2(K)=X2(K-1)+.3
      DO 22 J=2,11
      TH2(K,J)=(1065.+3.986*X2(K)-4.594*X1(J))/(5.685*(X1(J)-X2(K)))
      G2X2(K,J)=76.16*C3*(1.+TH2(K,J))*(.952*(1.+TH2(K,J))*(1065.-.608*
     1X2(K))-QDF*(5.685*TH2(K,J)+4.594))/U2AV/(41.*QDF*(5.685*TH2(K,J)+
     24.594)-.952*(1.+TH2(K,J))*(1432.5-.608*X2(K)+454.8*TH2(K,J)))
      SG12(K,J)=G2X2(K,J)+F1X1(J)
      IF(J-2)23,23,24
   23 F2X2(K)=SG12(K,J)
      PUNCH 13,X2(K),TH2(K,J),X1(J),G2X2(K,J),F1X1(J),F2X2(K)
   24 IF(F2X2(K)-SG12(K,J))22,22,26
   26 F2X2(K)=SG12(K,J)
      PUNCH 13,X2(K),TH2(K,J),X1(J),G2X2(K,J),F1X1(J),F2X2(K)
   22 CONTINUE
   21 CONTINUE
```

(Cont'd)

```
      CALC.TH3(L,K),F3X3(L)
      X3(1)=89.5
      DO 31 L=2,11
      X3(L)=X3(L-1)+.5
      DO 32 K=2,11
      TH3(L,K)=(1065.+2.986*X3(L)-3.594*X2(K))/(5.58*(X2(K)-X3(L)))
      G3X3(L,K)=75.2*C3*(1.+TH3(L,K))*(.94*(1.+TH3(L,K))*(1065.-.608*X3
     1(L))-QDF*(5.58*TH3(L,K)+3.594))/U3AV/(41.*QDF*(5.58*TH3(L,K) 3.594
     2)-.94*(1.+TH3(L,K))*(1352.5-.608*X3(L)+446.4*TH3(L,K)))+7.52*C3*(
     31.+TH3(L,K))/U3AV/(1.+1.88*QDF*(1.+TH3(L,K))*X3(L) -1.88*QDF*(1.+
     4TH3(L,K))*(TF+4.))
      SG23(L,K)=G3X3(L,K)+F2X2(K)
      IF(K-2)33,33,34
   33 F3X3(L)=SG23(L,K)
      PUNCH 13,X3(L),TH3(L,K),X2(K),G3X3(L,K),F2X2(K),F3X3(L)
   34 IF(F3X3(L)-SG23(L,K))32,32,36
   36 F3X3(L)=SG23(L,K)
      PUNCH 13,X3(L),TH3(L,K),X2(K),G3X3(L,K),F2X2(K),F3X3(L)
   32 CONTINUE
   31 CONTINUE
      END
```

TABLE 3

ONE STAGE OPTIMAL TABLE

$(x_1^0 = 250,\ q/F = 26.7)$				$(x_1^0 = 250,\ q/F = 27.0)$			
x_1^1 °F	θ^1 lb/lb	$G^1(x_1^1;\theta^1)$ x 10^5 $/lb	$f_1(x_1^1)$ x 10^5 $/lb	x_1^1 °F	θ^1 lb/lb	$G^1(x_1^1;\theta^1)$ x 10^5 $/lb	$f_1(x_1^1)$ x 10^5 $/lb
201.7	2.42	1.69001	1.69001	201.7	2.42	1.70145	1.70145
202.0	2.44	1.69194	1.69194	202.0	2.44	1.70334	1.70334
202.3	2.46	1.69391	1.69391	202.3	2.46	1.70525	1.70525
202.6	2.48	1.69591	1.69591	202.6	2.48	1.70720	1.70720
202.9	2.50	1.69794	1.69794	202.9	2.50	1.70919	1.70919
203.2	2.52	1.70002	1.70002	203.2	2.52	1.71121	1.71121
203.5	2.54	1.70213	1.70213	203.5	2.54	1.71326	1.71326
203.8	2.57	1.70427	1.70427	203.8	2.57	1.71535	1.71535
204.1	2.59	1.70646	1.70646	204.1	2.59	1.71748	1.71748
204.4	2.61	1.70868	1.70868	204.4	2.61	1.71965	1.71965

TABLE 3 (Cont'd)

ONE STAGE OPTIMAL TABLE

$(x_1^0 = 250,\ q/F = 27.3)$				$(x_1^0 = 250,\ q/F = 27.6)$			
x_1^1	θ^1	$G^1(x_1^1;\theta^1)$ x 10^5	$f_1(x_1^1)$ x 10^5	x_1^1	θ^1	$G^1(x_1^1;\theta^1)$ x 10^5	$f_1(x_1^1)$ x 10
°F	lb/lb	$/lb	$/lb	°F	lb/lb	$/lb	$/lb
201.7	2.42	1.71307	1.71307	201.7	2.42	1.72484	1.7248
202.0	2.44	1.71491	1.71491	202.0	2.44	1.72664	1.7266
202.3	2.46	1.71677	1.71677	202.3	2.46	1.72846	1.7284
202.6	2.48	1.71868	1.71868	202.6	2.48	1.73032	1.7303
202.9	2.50	1.72061	1.72061	202.9	2.50	1.73220	1.7322
203.2	2.52	1.72258	1.72258	203.2	2.52	1.73412	1.7341
203.5	2.54	1.72458	1.72458	203.5	2.54	1.73608	1.7360
203.8	2.57	1.72662	1.72662	203.8	2.57	1.73807	1.7380
204.1	2.59	1.72870	1.72870	204.1	2.59	1.74009	1.7400
204.4	2.61	1.73081	1.73081	204.4	2.61	1.74215	1.7421

TABLE 3 (Cont'd)

ONE STAGE OPTIMAL TABLE

($x_1^0 = 250$, $q/F = 27.9$)

x_1^1	θ^1	$G^1(x_1^1;\theta^1)$	$f_1(x_1^1)$
		x 10^5	x 10^5
^oF	lb/lb	\$/lb	\$/lb
201.7	2.42	1.73677	1.73677
202.0	2.44	1.73852	1.73852
202.3	2.46	1.74030	1.74030
202.6	2.48	1.74211	1.74211
202.9	2.50	1.74395	1.74395
203.2	2.52	1.74583	1.74583
203.5	2.54	1.74774	1.74774
203.8	2.57	1.74968	1.74968
204.1	2.59	1.75165	1.75165
204.4	2.61	1.75366	1.75366

TABLE 4

TWO STAGE OPTIMAL TABLE

$q/F = 26.7$

x^2 °F	θ^2 lb/lb	$G^2(x_1^2;\theta^2)$ x 10^6 \$/lb	x^1 °F	$f_1(x_1^1)$ x 10^5 \$/lb	$f_2(x_1^2)$ x 10^5 \$/lb
148.8	2.43	2.7190	201.7	1.69000	1.96191
149.1	2.45	2.7368	201.7	1.69000	1.96370
149.4	2.44	2.7354	202.0	1.69194	1.96549
149.7	2.46	2.7536	202.0	1.69194	1.96730
150.0	2.46	2.7522	202.3	1.69391	1.96913
150.3	2.48	2.7706	202.3	1.69391	1.97097
150.6	2.48	2.7692	202.6	1.69591	1.97283
150.9	2.50	2.7878	202.6	1.67591	1.97470
151.2	2.50	2.7864	202.9	1.69794	1.97659
151.5	2.52	2.8054	202.9	1.69794	1.97849

TABLE 4 (Cont'd)

TWO STAGE OPTIMAL TABLE

q/F = 27.0

x_1^2 °F	θ^2 lb/lb	$G^2(x_1^2;\theta^2)$ x 10^6 $/lb	x_1^1 °F	$f_1(x_1^1)$ x 10^5 $/lb	$f_2(x_1^2)$ x 10^5 $/lb
148.8	2.43	2.6638	201.7	1.70145	1.96784
149.1	2.45	2.6812	201.7	1.70145	1.96958
149.4	2.44	2.6798	202.0	1.70334	1.97133
149.7	2.46	2.6975	202.0	1.70334	1.97309
150.0	2.46	2.6961	202.3	1.70525	1.97487
150.3	2.48	2.7140	202.3	1.70525	1.97666
150.6	2.48	2.7127	202.6	1.70720	1.97848
150.9	2.50	2.7309	202.6	1.70720	1.98030
151.2	2.50	2.7295	202.9	1.70919	1.98214
151.5	2.52	2.7480	202.9	1.70919	1.98399

TABLE 4 (Cont'd)

TWO STAGE OPTIMAL TABLE

q/F = 27.3

x_1^2 °F	θ^2 lb/lb	$G^2(x_1^2;\theta^2)$ x 10^6 $/lb	x_1^1 °F	$f_1(x_1^1)$ x 10^5 $/lb	$f_2(x_1^2)$ x 10^5 $/lb
148.8	2.43	2.6106	201.7	1.71307	1.97413
149.1	2.45	2.6275	201.7	1.71307	1.97582
149.4	2.45	2.6275	202.0	1.71491	1.97753
149.7	2.46	2.6434	202.0	1.71491	1.97925
150.0	2.46	2.6421	202.3	1.71677	1.98099
150.3	2.48	2.6595	202.3	1.71677	1.98273
150.6	2.48	2.6582	202.6	1.71868	1.98450
150.9	2.50	2.6759	202.6	1.71868	1.98627
151.2	2.50	2.6796	202.9	1.72061	1.98897
151.5	2.52	2.6926	202.9	1.72061	1.98987

TABLE 4 (Cont'd)

TWO STAGE OPTIMAL TABLE

$q/F = 27.6$

x_1^2 °F	θ^2 lb/lb	$G^2(x_1^2;\theta^2)$ x 10^6 $/lb	x_1^1 °F	$f_1(x_1^1)$ x 10^5 $/lb	$f_2(x_1^2)$ x 10^5 $/lb
148.8	2.43	2.5592	201.7	1.72484	1.98077
149.1	2.45	2.5758	201.7	1.72484	1.98242
144.4	2.44	2.5745	202.0	1.72484	1.98404
149.7	2.46	2.5912	202.0	1.72664	1.98577
150.0	2.46	2.5900	202.3	1.72846	1.98746
150.3	2.48	2.6070	202.3	1.72846	1.98916
150.6	2.48	2.6057	202.6	1.73032	1.99089
150.9	2.50	2.6230	202.6	1.73032	1.99262
151.2	2.52	2.6405	202.6	1.73032	1.99437
152.5	2.52	2.6392	202.9	1.73220	1.99613

TABLE 4 (Cont'd)

TWO STAGE OPTIMAL TABLE

q/F = 27.9

x_1^2 °F	θ^2 lb/lb	$G^2(x_1^2;\theta^2)$ x 10^6 $/lb	x_1^1 °F	$f_1(x_1^1)$ x 10^5 $/lb	$f_2(x_1^2)$ x 10^5 $/lb
148.8	2.43	2.5097	201.7	1.73677	1.98774
149.1	2.45	2.5422	201.7	1.73677	1.99099
149.4	2.44	2.5245	202.0	1.73852	1.99098
149.7	2.46	2.5409	202.0	1.73852	1.99262
150.0	2.46	2.5396	202.3	1.74030	1.99427
150.3	2.48	2.5563	202.3	1.74030	1.99593
150.6	2.48	2.5550	202.6	1.74211	1.99762
150.9	2.50	2.5718	202.6	1.74030	1.99930
151.2	2.52	2.5890	202.6	1.74211	2.00101
151.5	2.52	2.5877	202.9	1.74395	2.00273

TABLE 5

THREE STAGE OPTIMAL TABLE

$q/F = 26.7$

x_1^3 °F	θ^3 lb/lb	$G^3(x_1^3;\theta^3)$ x 10^6 $/lb	x_1^2 °F	$f_2(x_1^2)$ x 10^5 $/lb	$f_3(x_1^3)$ x 10^5 $/lb
90.0	2.43	3.1013	148.8	1.96191	2.27205
90.5	2.46	3.1260	148.8	1.96191	2.27451
91.0	2.47	3.1343	149.1	1.96370	2.27713
91.5	2.48	3.1432	149.4	1.96549	2.27981
92.0	2.48	3.1524	149.7	1.96730	2.28255
92.5	2.49	3.1619	150.0	1.96913	2.28532
93.0	2.50	3.1715	150.3	1.97097	2.28812
93.5	2.52	3.1813	150.6	1.97283	2.29096
94.0	2.53	3.1912	150.9	1.97470	2.29382
94.5	2.54	3.2012	151.2	1.97659	2.29672

TABLE 5 (Cont'd)

THREE STAGE OPTIMAL TABLE

q/F = 27.0

x_1^3 °F	θ^3 lb/lb	$G^3(x_1^3;\theta^3)$ x 10^6 $/lb	x_1^2 °F	$f_2(x_1^2)$ x 10^5 $/lb	$f_3(x_1^3)$ x 10^5 $/lb
90.0	2.43	3.0379	148.8	1.96784	2.27163
90.5	2.46	3.0618	148.8	1.96784	2.27403
91.0	2.47	3.0699	149.1	1.96958	2.27657
91.5	2.48	3.0963	149.4	1.97133	2.27919
92.0	2.48	3.0875	199.7	1.97309	2.28185
92.5	2.49	3.0967	150.0	1.97487	2.28455
93.0	2.50	3.1061	150.3	1.97666	2.28728
93.5	2.52	3.1156	150.6	1.97848	2.29004
94.0	2.53	3.1438	150.9	1.98030	2.29283
94.5	2.59	3.1350	151.2	1.98214	2.29565

TABLE 5 (Cont'd)

THREE STAGE OPTIMAL TABLE

$q/F = 27.3$

x_1^3	θ^3	$G^3(x_1^3;\theta^3)$ x 10^6	x_1^2	$f_2(x_1^2)$ x 10^5	$f_3(x_1^3)$ x 10^5
^oF	lb/lb	\$/lb	^oF	\$/lb	\$/lb
90.0	2.43	2.9768	148.8	1.97413	2.27181
90.5	2.46	3.0001	148.8	1.97413	2.27414
91.0	2.47	3.0079	149.1	1.97582	2.27662
91.5	2.48	3.0163	149.4	1.97753	2.27917
92.0	2.48	3.0251	149.7	1.97925	2.28176
92.5	2.49	3.0340	150.0	1.98099	2.28434
93.0	2.50	3.0431	150.3	1.98273	2.28705
93.5	2.52	3.0524	150.6	1.98450	2.28775
94.0	2.53	3.0618	150.9	1.98627	2.29296
94.5	2.54	3.0713	151.2	1.98807	2.29521

TABLE 5 (Cont'd)

THREE STAGE OPTIMAL TABLE

$q/F = 27.6$

x_1^3	θ^3	$G^3(x_1^3;\theta^3)$	x_1^2	$f_2(x_1^2)$	$f_3(x_1^3)$
		$\times 10^6$		$\times 10^5$	$\times 10^5$
^oF	lb/lb	\$/lb	^oF	\$/lb	\$/lb
90.0	2.43	2.9179	148.8	1.98077	2.27256
90.5	2.46	2.9405	148.8	1.98077	2.27483
91.0	2.47	2.9482	149.1	1.98242	2.27725
91.5	2.48	2.9564	149.4	1.98409	2.27973
92.0	2.48	2.9649	149.7	1.98577	2.28226
92.5	2.49	2.9736	150.0	1.98746	2.28482
93.0	2.50	2.9829	150.3	1.98916	2.28741
93.5	2.52	2.9915	150.6	1.99089	2.29004
94.0	2.53	3.0006	150.9	1.99262	2.29268
94.5	2.54	3.0099	151.2	1.99437	2.29536

TABLE 5 (Cont'd)

THREE STAGE OPTIMAL TABLE

$q/F = 27.9$

x_1^3 °F	θ^3 lb/lb	$G^3(x_1^3;\theta^3)$ x 10^6 $/lb	x_1^2 °F	$f_2(x_1^2)$ x 10^5 $/lb	$f_3(x_1^3)$ x 10^5 $/lb
90.0	2.43	2.8611	148.8	1.98774	2.27385
90.5	2.46	2.8831	148.8	1.98774	2.27606
91.0	2.47	2.8906	149.1	1.98936	2.27892
91.5	2.48	2.8985	149.4	1.99098	2.28084
92.0	2.48	2.9068	149.7	1.99262	2.28330
92.5	2.49	2.9153	150.0	1.99427	2.28580
93.0	2.50	2.9239	150.3	1.99593	2.28833
93.5	2.52	2.9327	150.6	1.99762	2.29089
94.0	2.53	2.9416	150.9	1.99930	2.29397
94.5	2.54	2.9506	151.2	2.00101	2.29608

Conclusion:

(1) Optimal path

x_1^0, θ^1, x_1^1, θ^2, x_1^2, θ^3, x_1^3

250.0, 2.42, 201.7, 2.45, 149.1, 2.47, 91.0

(2) $q/F = 27.1$

(3) Optimal production cost: $2.27654/lb distillate

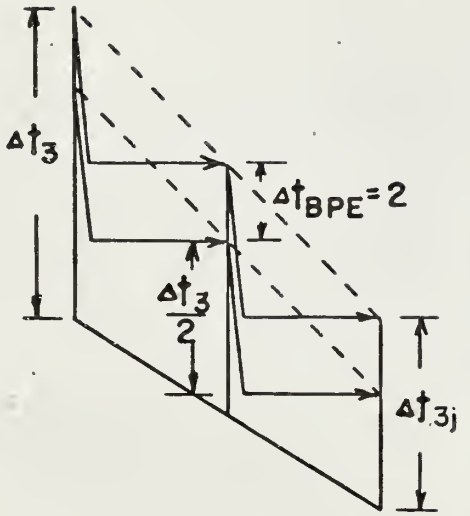


Fig. 5. Temperature profiles of the flashing brine, distillate and make-up feed + coolant in the heat rejection section of the third effect.

rejection section.

Δt_{3j} = temperature difference between the spent and make-up brine.

For this reason, if a make-up feed of 85°F is used, the flashing brine temperature should be at least 89°F. Actually, from the mechanical point of view, there is a restriction on the final blowdown temperature because there is a limitation to the highest vacuum maintainable.

From the computed results we can see that, for a final blowdown temperature, x_1^3, below 91°F, the production cost is strictly monotonically decreasing, but this does not necessarily guarantee that the production cost is really decreasing because we have not included the pumping cost of the coolant in this study. If we take an energy balance for the heat rejection section of the third effect, the following approximate relationship holds.

$$F(1+r_3)(C_p)_{f3}\Delta t_{3r} = F(1+r_c)(C_p)_F\Delta t_{3j} .$$

Since $(C_p)_{f3} \doteq (C_p)_F$ and r_3 is of the magnitude of 2.5, we have, by taking $\Delta t_{3r} = 8$ and $\Delta t_{3j} = 4$

$$8(1+r_3) = (1+r_c)4$$

$$r_c = 2r_3 + 1 \doteq 6 .$$

where r_c is the ratio of the coolant and make-up feed. It is seen that a large quantity of coolant is required and hence, there is an increase in the pumping cost as the blowdown temperature decreases which we did not take into account.

It is concluded that the decrease in production cost by lowering the final blowdown temperature does not necessarily compensate for the increase due to the pumping cost of the coolant. Therefore, it would probably be

better that the final blowdown temperature be fixed at $91^{o}F$ or slightly above this.

In Fig. 6 a plot of the production cost vs q/F is given using the final blowdown temperature x_1^3 as a parameter. It is seen that there is a minimum point corresponding to each final blowdown temperature and that it shifts in the direction of decreasing q/F as the final blowdown temperature decreases. From Fig. 7, it can be seen that the optimal value of q/F is located at a point approximately equal to 27.1 and that the corresponding optimal production cost is equal to $\$2.27654 \times 10^{-5}$/lb. It is to be noted that there is a minor error involved in this estimation due to the discretization of the grid points which is inherent in dynamic programming. A value more accurate than this for the optimal production cost can be obtained by linear interpolation. Since the production cost curve is so flat, this interpolation was not carried out here.

Finally, we add the general expenses and administrative expenditures of $\$0.172/10^3$ gallons so that the optimal value of the total production cost, $\$0.3993/10^3$ gallons, or approximately $\$0.4/10^3$ gallons at q/F of 27.1, can be obtained.

In Fig. 8, the production costs are plotted against the final blowdown temperatures at the computed optimal value of q/F = 27.0, which is closest to the true optimal value of q/F = 27.1. It shows that the production cost is approximately a linear function of the final blowdown temperature for a given q/F. This is consistent with the fact that for a given heat input to the system, the lower the final blowdown temperature, the better the heat economy and the lower the production cost. In Fig. 8, a plot of the production cost vs. the second blowdown temperature x_1^2 is also given with x_1^1

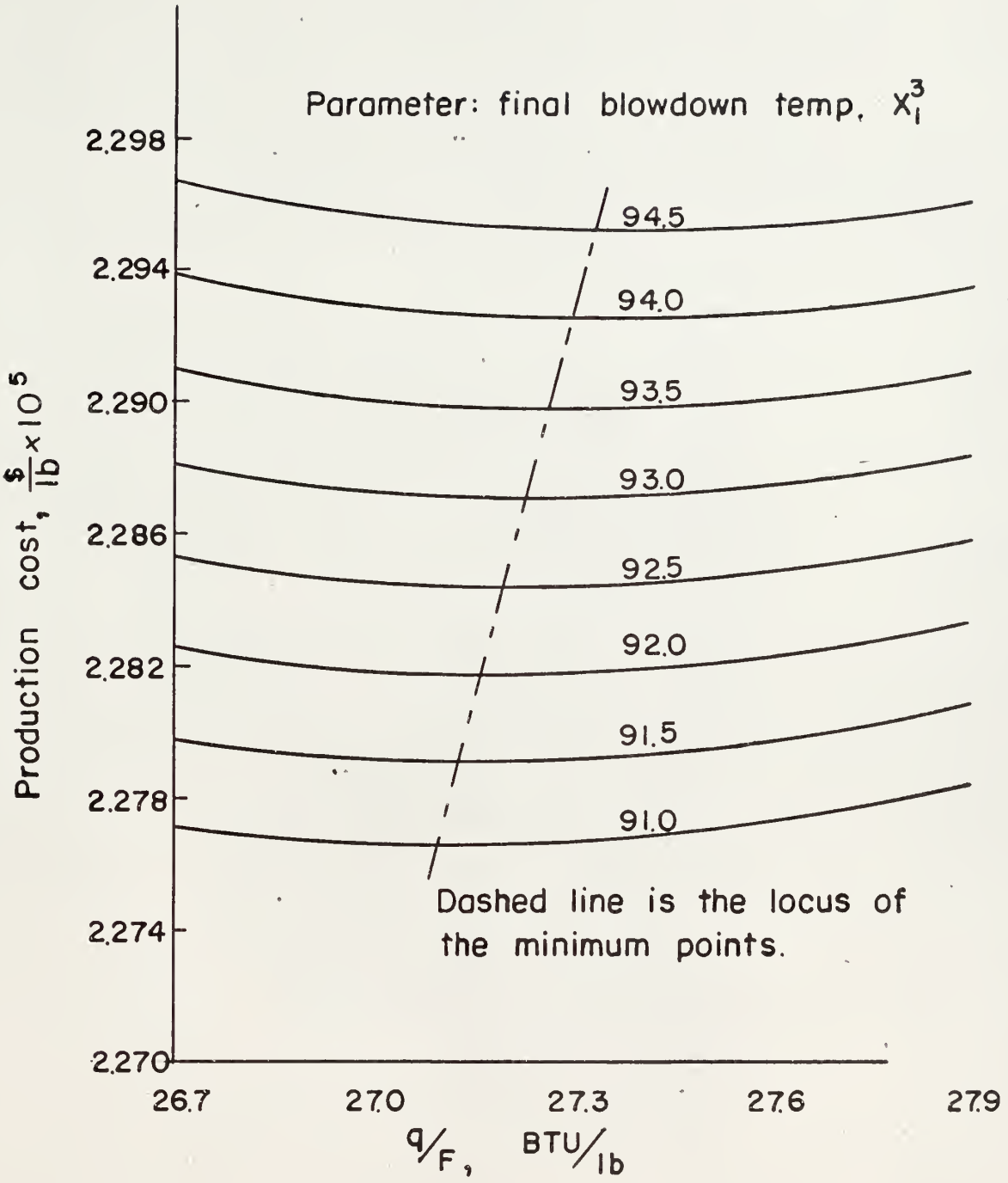


Fig. 6. Production cost vs. the ratio of energy input to the make-up feed with the final blowdown temperature X_1^3 as parameter.

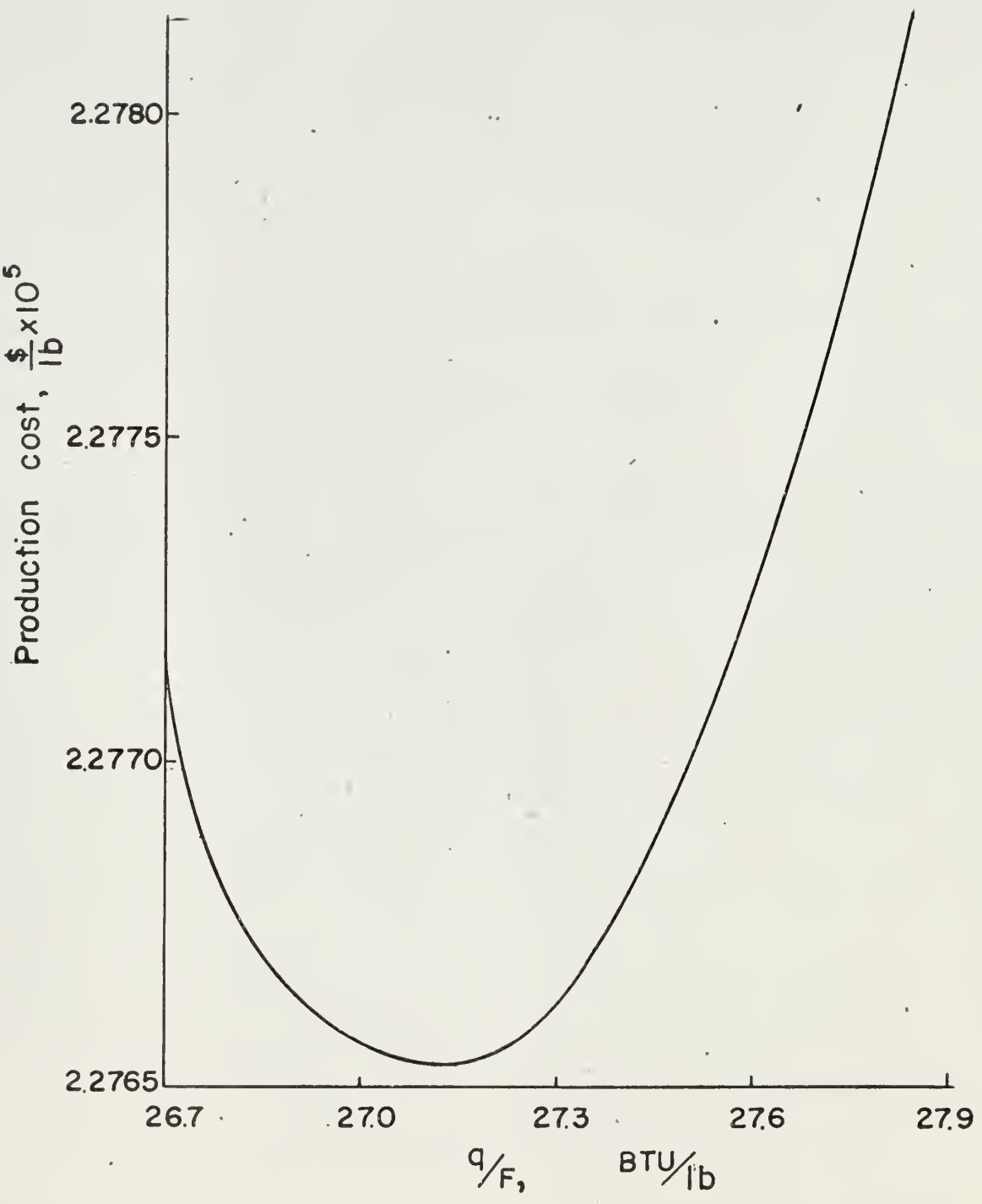


Fig. 7. Production cost plotted against the ratio of energy imput to the make-up feed with the final blowdown temperature $X_1^3 = 91\ ^\circ F$.

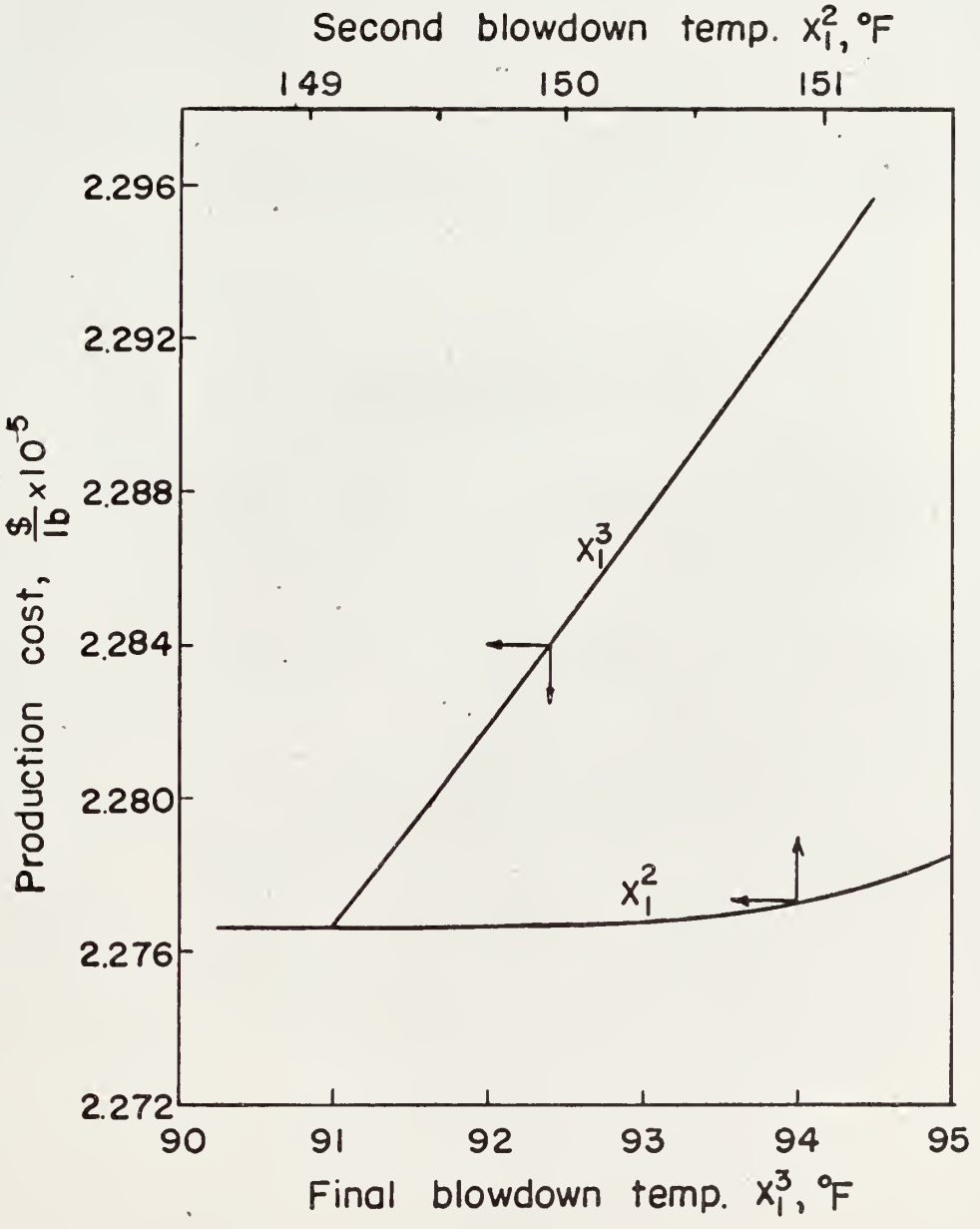


Fig.8. Production cost vs. final blowdown temperature x_1^3, and vs. second blowdown temperature x_1^2 with x_1^1 = 201.7, x_1^3=91 and $9/F$=27.

and x_1^3 fixed in the optimal path of 201.7°F and 91.0°F respectively. The optimal production costs in both plots agree with each other.

In Table 6, comparison of the production cost among cases with optimal and non-optimal policies is given. The optimal production cost is equal to $\$0.2273/10^3$ gallon. There is another case which gives the same value due to the truncation error.

REFERENCES

1. The Fluor Corporation, "Computational Design Study on 50 Million Gallon per Day MSM Desalination Plant for Office of Saline Water, U. S. Department of the Interior" Final Report, Jan. 1965.
2. Bechtel Corporation, "Cost Studies of Large Multi-Stage Flash Saline Water Conversion Plants for Office of Saline Water," Research and Development Program Report No. 116, Oct. 1964.
3. Roberts, S. M., "Dynamic Programming in Chemical Engineering and Process Control," Academic Press, New York, 1964.

TABLE 6

COMPARISON OF THE PRODUCTION COST AMONG THE CASES WITH OPTIMAL AND NON-OPTIMAL POLICIES

q/F	x_1^0	θ^1	x_1^1	θ^2	x_1^2	θ^3	x_1^3	Production cost
Results of the optimal policy by D. P.								
27.1	250	2.42	201.7	2.45	149.1	2.47	91.0	0.2273
Results of the non-optimal policy by P. P.								
27.0	250	2.44	202.0	2.44	149.4	2.48	91.5	0.2277
27.0	250	2.46	202.3	2.46	150.0	2.49	92.5	0.2281
27.0	250	2.42	201.7	2.46	149.4	2.48	91.5	0.2275
27.0	250	2.42	201.7	2.43	148.8	2.48	91.0	0.2273+*
27.0	250	2.44	202.0	2.44	149.4	2.48	91.5	0.2276
27.0	250	2.44	202.0	2.48	150.0	2.49	92.5	0.2281
Results of simulation								
	x_1^0	θ^1	x_1^1	θ^2	x_1^2	θ^3	x_1^3	Production cost ($/10^3$ gallon)
26.4	250	2.441	202.0	2.523	150.6	2.613	95.2	0.2417
31.0	250	2.585	204.0	2.481	152.0	2.350	91.6	0.2453
31.0	250	2.585	204.0	2.481	152.0	2.369	92.0	0.2419

*This is due to the truncation error in the computer printing.

NOMENCLATURE

c_1	Unit steam cost,	$\frac{\$}{lb.}$
c_2	Unit fixed charge cost, brine heater,	$\frac{\$}{ft^2,hr.}$
c_3	Unit fixed charge cost, condenser tubes,	$\frac{\$}{ft^2,hr.}$
c_4	Unit pumping cost,	$\frac{\$}{HPhr}$
$f_1(x_1^1)$	Maximum return function, one-stage process,	$\frac{\$}{lb}$
$f_2(x_1^2)$	Maximum return function, two-stage process,	$\frac{\$}{lb}$
$f_3(x_1^3)$	Maximum return function, three-stage process,	$\frac{\$}{lb}$
$G(x_1^1;\theta^1)$	Return function, stage 1,	$\frac{\$}{lb}$
$G^2(x_1^2;\theta^2)$	Return function, stage 2,	$\frac{\$}{lb}$
$G^3(x_1^3;\theta^3)$	Return function, stage 3,	$\frac{\$}{lb}$
$\frac{q}{F}$	Ratio of the energy input to the make-up feed,	$\frac{lb}{lb}$
T_F	Temperature of the make-up feed,	^oF
U_B	Overall heat transfer coefficient of the heater tubes,	$\frac{BTU}{ft^2\text{-}hr}$
$(U_n)_{av}$	Overall heat transfer coefficient of the condenser tubes, subscript n is the stage number,	$\frac{BTU}{ft^2.hr}$
x_1	Blowdown temperature of the first stage,	^oF
x_2	Blowdown temperature of the second stage,	^oF

x_3	Blowdown temperature of the third stage,	^oF

Greek Letters

s	Latent heat of process steam,	$\frac{BTU}{lb}$
θ^n	Ratio of the recycle brine to the make-up feed, superscript is the stage number,	$\frac{lb}{lb}$

CHAPTER IV

REFINEMENT OF SOLUTIONS AND REDUCTION IN DIMENSIONALITY

As stated in Chapter I, the main disadvantage of dynamic programming is the dimensionality difficulty which occurs as the number of state variables increases. Various schemes have been proposed to overcome the dimensionality difficulty [1, 2, 3, 4]. Most of them essentially trade computer time for computer memory. One way of reducing the memory requirement is to increase the interval size, or to decrease the number of grid points. But the discretization error will be magnified and hence there results a solution which is not very accurate. Either linear interpolation or extrapolation must be used to refine the solution for the case in which the transformation functions are almost linear or only approximate solutions are desired. Furthermore, iteration can also be used to obtain more accurate results.

In this chapter, a more sophisticated interpolation technique, namely the polynomial approximation, and several methods for reducing the dimensionality of a process such as the use of the Lagrangian multipliers, the ratio of state variables and the method of continuous independent variable are presented.

1. POLYNOMIAL APPROXIMATION

Instead of listing a table of grid points for the state variables, the table which represents the maximum return function $f_{N-1}(x)$ is correlated into a polynomial during the computations [2]. Thus each polynomial stands for a maximum return function, $f_n(x)$, for $n = 1,\ldots, N$. In the present approach, we shall use the least-square method and represent the optimal table by means of orthogonal Legendre polynomials

$$f_n(x) = \sum_{K=0}^{R} a_{Kn} P_K(x) . \tag{1}$$

The function $f_n(x)$ is a polynomial of degree R, and $P_K(x)$ is a polynomial of degree K on the interval $[-1, 1]$.

From the orthogonal properties of these polynomials

$$\int_{-1}^{1} P_k(x) P_j(x) dx = \begin{cases} 0 & k \neq j \\ \dfrac{2}{2k+1} & k = j \end{cases}$$

one is able to obtain

$$a_{kn} = \frac{2k+1}{2} \int_{-1}^{1} f_n(x) P_k(x) dx . \tag{2}$$

The integration on the right of equation (2) may be performed by use of Gaussian quadrature

$$\int_{-1}^{1} f_n(x) P_k(x) dx = \sum_{j=1}^{s} b_j f_n(x_j) P_k(x_j) \tag{3}$$

which is exact when $f_n(x) P_k(x)$ is a polynomial of degree 2s-1, and the x_j's are the zeros of the Legendre polynomial of degree s and the b_j's are the Christoffel numbers (weights). For this functional approximation and integration the optimum grid spacing is not equidistant and we require the storage of R+1 coefficients [4].

Now, we consider the system with the following functional equations

$$f_1(c) = \max_{\theta} g(c;\theta)$$

$$f_N(c) = \max_{\theta} \left\{ g(c;\theta) + f_{N-1}(T(c;\theta)) \right\} \tag{4}$$

where c is the initial state and $T(c;\theta)$ is the transformation equation.

In order to obtain $f_n(x_j)$ we must first evaluate $f_1(x_j)$ for $x_1, x_2, \ldots, x_s$, the zeros of the Legendre polynomial of degree s. We evaluate $f_1(x_j)$ as usual for a one-stage process by the proper choice of θ; with the value of $f_1(x_j)$ obtained, we evaluate $f_1(x)$ for any value of x in the range of (-1, 1). The b_j and $P_k(x_j)$ are found from tables or the Legendre polynomial recursion equations. Then $a_{k,1}$ is found for $k = 1, 2, \ldots, R$. Once the $a_{k,1}$ are known, we can evaluate $f_1(x)$ for any x within (-1, 1). In such a manner, $f_1(x)$ is curve fitted from the values of the $f_1(x_j)$ terms.

For the two-stage process, we evaluate $f_2(x_j)$ by equation (4). The choice of the θ that maximizes the right hand side of equation (4) transforms the state of the system from x_j into $(x_j + \Delta x_j)$. Since the new state $x_j + \Delta x_j$ will, in general, not be a zero of the Legendre polynomial of degree s, the term $f_1(x_j + \Delta x_j)$ can be evaluated from the coefficients $a_{k,1}$, which were developed from the one-stage process. The coefficients $a_{k,2}$, $k = 0, 1, \ldots, R$ can be obtained from equation (3) as soon as $f_2(x_j)$ are evaluated. From $a_{k,2}$ and equation (1), $f_2(x)$ is found for general values of x. Again, $f_2(x)$ is curve fitted from $f_2(x_j)$. In this manner, we develop $f_N(x)$. It is noted that the Legendre polynomials $P_k(x_j)$ and the coefficient b_j can be calculated independently of $f_N(x_j)$ [5].

The following is an outline of this scheme applied to the optimum allocation of residence time in a continuous stirred tank reactor system.

Let us consider an isothermal first order reversible reaction

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$$

carried out in a sequence of three CSTR's as shown in Fig. 1.

We take

k_1 = forward reaction rate = 1.19, min^{-1}

k_2 = backward reaction rate = 0.02, min^{-1}

c_e = equilibrium concentration of B = 0.95, lb-mole/ft^3

r = final concentration of B = 0.9, lb-mole/ft^3.

Our objective is to minimize the total residence time by proper choice of θ_n, n = 1, 2 (θ_3 is fixed since the final concentration of B is given).

According to [6], the least total holding time required for an N-stage process is

$$f_N(c_{N+1}) = \frac{N}{k_1 + k_2}\left[\left(\frac{c_e - c_{N+1}}{c_e - r}\right)^{1/N} - 1\right]$$

where c_{N+1} is the initial concentration of B. We shall consider the case $c_{N+1} = 0$, and perform the approximation by use of a Legendre polynomial of degree 3.

Then it takes the form

$$f_n(c) = \sum_{k=0}^{3} a_{kn} P_k(c)$$

since the interval of c is $0 \leqslant c \leqslant 0.9$, we have to transform the interval of integration by the formula (7)

$$c = \frac{(b-a)x + b + a}{2}$$

in which $-1 \leqslant x \leqslant 1$, and $a \leqslant c \leqslant b$. In this case a = 0, b = 0.9, so that

$$c = \frac{0.9x + 0.9}{2} = 0.45(x+1)$$

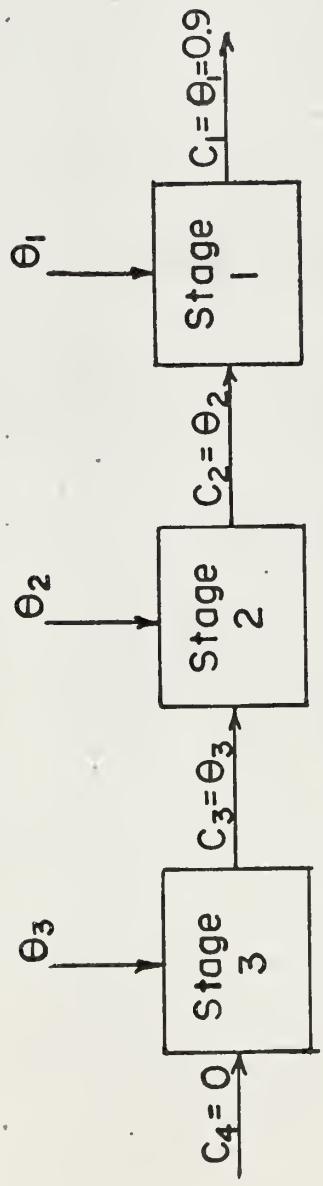


Fig. 1. Schematic diagram for an isothermal, first-order, reversible reaction $A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$.

or

$$x = \frac{c - 0.45}{0.45}$$

The corresponding polynomials

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 + 1)$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

are transformed into functions of c.

Since we take K = 3, s = 4 will give an exact formulation. Starting with a one stage process, we write

$$f_1(c_2) = \sum_{k=0}^{3} a_{k,1} P_k(c_2)$$

$$f_n(c) = \sum_{k=0}^{3} a_{kn} P_k(c) .$$

Since the interval of c is $0 \leqq c \leqq 0.9$, we have to transform the interval of integration by the formula (7)

$$c = \frac{(b-a)x + b + a}{2}$$

in which $-1 \leqq x \leqq 1$, and $a \leqq c \leqq b$. In our case a = 0, b = 0.9, so that

$$c = \frac{0.9x + 0.9}{2} = 0.45(x+1)$$

or

$$x = \frac{c - 0.45}{0.45} .$$

The procedure is:

1. Find the roots x_j and weights b_j of the Legendre polynomial of degree 4 from a mathematical table ($j = 1, 2, 3, 4$).

2. Transform $P_k(x)$ to $P_k(c_2)$ by $x = \frac{c_2 - 0.45}{0.45}$ for $k = 0, 1, 2, 3$.

3. Evaluate $P_k(c_{2j})$

$$c_{2j} = 0.45(x_j + 1) .$$

4. Evaluate $f_1(c_{2j})$.

5. Replace b_j by $0.45b_j$ for change in interval from $-1 \leq x \leq 1$ to $0 \leq c_2 \leq 0.9$.

6. Evaluate a_{k1} by

$$a_{k1} = \frac{2k+1}{2} \sum_{j=1}^{4} b_j f_1(c_{2j}) P_k(c_{2j}) , \qquad k = 0, 1, 2, 3 .$$

7. Find $f_1(c_2)$ for any value of c_2.

For a two-stage process, we can proceed in the same manner.

Since the functional equation is of the form

$$f_2(c_3) = \min_{\theta_2} \left\{ g(c_3; \theta_2) + f_1(c_2) \right\}$$

or

$$f_2(c_{3j}) = \min_{\theta_{2j}} \left\{ g(c_{3j}; \theta_{2j}) + f_1(c_{3j} + \Delta c_{3j}) \right\}$$

we have to choose the optimal value of θ_{2j} corresponding to c_{3j} so that $f_2(c_{3j})$ are obtained for $j = 1, 2, 3, 4$.

It should be noted that the first and second label of the subscript are the stage and grid point number (root number of the Legendre polynomial) respectively.

2. LAGRANGIAN MULTIPLIERS

Lagrangian multipliers have been extensively used for the optimization of non-linear functions with some types of constraints. Aris [8] used the technique to consider constraints in dynamic programming problems. Kuo and Rubin [9] applied the method to determine inlet conditions of a process in order to extremize characteristics of the chemical reactions and simultaneously meet certain constraints such as specified product yield or temperature.

Let a function $f(x_1,\ldots, x_n)$ be minimized subject to the constraints

$$g_j(x_1,\ldots, x_n) = 0, \qquad j = 1,\ldots, m \qquad m \leq n . \tag{5}$$

Then, it is required to find the minima of

$$f(x_1,\ldots, x_n) + \sum_{j=1}^{M} \lambda_j g_j(x_1,\ldots, x_n) \tag{6}$$

where λ_j are called Lagrangian multipliers. This involves setting the partial derivatives of this function equal to zero, but this in itself is not a sufficient condition for a relative minimum. For example, in the case of $f(x_1, x_2) = x_1 x_2$, the origin is neither a minimum nor a maximum and is called a saddle point. In any case, setting the partial derivatives of this function equal to zero is a necessary condition for a stationary value of the function. The sufficient conditions for relative maxima and minima involve, in addition to the first partial derivative being zero, the

inequalities in the second order derivatives.

When the variables are constrained by inequalities rather than by equations, or by both types, then the Lagrange method cannot be directly applied. However, an appreciable extension has been developed by Kuhn and Tucker [10].

For the case of handling inequality constraints, such as $T_{min} \leqslant T \leqslant T_{max}$, we introduce so-called slack variables and let $u^2 = (T - T_{min})(T_{max} - T) \geqslant 0$, when $T = T_{min}$ or T_{max} $u^2 = 0$. This is suggested by Valentine [11].

Next, we will consider the formal application of the Lagrangian multipliers in the dynamic programming formulation. Suppose we wish to maximize a sum of N functions $\sum_{1}^{N} g_n(x_n)$ of the n positive variables $x_1, \ldots, x_N$, subject to restrictions such as

$$\sum_{n=1}^{N} k_{mn}(x_n) \leqslant k_m , \qquad m = 1, \ldots, M . \tag{7}$$

Then the maximum we obtain will be a function of the set of quantities k_m, and we write

$$\max \sum_{1}^{N} g_n(x_n) = f_N(k_1, \ldots, k_N) . \tag{8}$$

If we make an allocation x_N then the remaining allocations $x_{N-1}, \ldots, x_1$ are subject to

$$\sum_{n=1}^{N-1} k_{mn}(x_n) = K_m - k_{mN}(x_N) . \tag{9}$$

The maximum of $\sum_{1}^{N-1} g_n(x_n)$ subject to these restrictions is

$$f_{N-1}(K_1 - k_{1N}(x_N), \ldots, K_M - k_{MN}(x_N)) \ .$$

Thus writing

$$\sum_1^N g_n(x_n) = g_N(x_N) + \sum_1^{N-1} g_n(x_n)$$

and applying the principle of optimality, we have

$$f_N(K_1, \ldots, K_M) = \max \left[g_N(x_N) + f_{N-1}(K_1 - k_{1M}(x_N), \ldots, K_M - k_{MM}(x_M)) \right] . \qquad (10)$$

This is a typical dynamic programming formulation but its dimensionality is M and the storage requirements increase exponentially with M.

If we modify the objective function to

$$\sum_1^N g_n(x_n) - \lambda_M \sum_1^N k_{Mn}(x_n) \qquad (11)$$

we can solve the problem for fixed λ_M and consider only the first (M-1) restrictions in equation (7). Thus we can write

$$f_N(K_1, \ldots, K_{M-1}, \lambda_M) = \max \left[\sum_1^N \left\{ g_n(x_n) - \lambda_M k_{Mn}(x_n) \right\} \right] \qquad (12)$$

and its dimensions are only (M-1). When it has been solved, we have only to find the λ_M which satisfies the condition in (6). In general, we can eliminate the (M-1) restrictions by introducing Lagrangian multipliers and write

$$f_N(K_1, \ldots, K_L; \lambda_{L+1}, \ldots, \lambda_M) = \max \sum_1^N \left[g_n(x_n) - \sum_{L+1}^N \lambda_m k_{mn}(x_n) \right] \qquad (13)$$

We now have dimension L but must look for the set of (M-L) Lagrangian

multipliers that satisfy the last (M-L) restrictions. This is in effect, exchanging computer memory for time.

In regard to the physical significance of the Lagrangian multiplier, one may consider it the operating cost per unit volume for the CSTR sequence when one considers the optimal allocation of the reactor volume or equivalently of the residence (or holding) time with restriction on the total volume [6].

A Lagrangian multiplier may also be interpreted as the relative cost or cost ratio when one considers the allocation of a limited resource, an illustrative example using a Lagrangian multiplier will be presented in Chapter VI for the solvent allocated to the cross-current extraction system with a recycle loop.

3. RATIOS OF STATE VARIABLES

If the transformation functions of the state variables are homogeneous in nature and are linear with respect to each other, this linear property simplifies the problem in that the ratio of two state variables may be used as a new state variable. This reduces the dimensionality difficulty in that it results in a reduction in the number of state variables [8].

As an illustration, let us consider an isothermal first order consecutive reaction,

$$A \xrightarrow{k_1 = 0.1} R \xrightarrow{k_2 = 0.1} S,$$

carried out in a series of N CSTR as shown in Fig. 2. If we define

x_1^n = concentration of species A at stage n

x_2^n = concentration of species R at stage n

then the reaction rates of A and R are

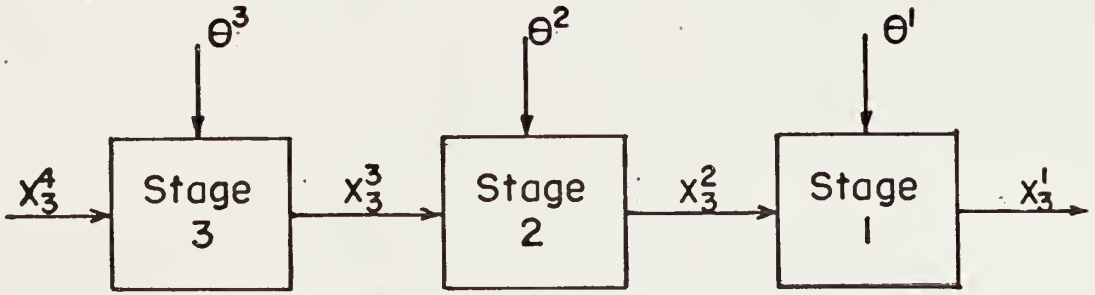


Fig. 2. Schematic diagram for an isothermal, first-order, consecutive reaction $A \xrightarrow{k_1} R \xrightarrow{k_2} S$.

$$(-r_A^n) = k_1 x_1^n$$

$$(-r_R^n) = k_2 x_2^n - k_1 x_1^n \ .$$

The material balance of each species at stage n is

$$v x_1^{n+1} = v x_1^n + (-r_A^n) V^n$$

or

$$x_1^{n+1} = x_1^n + 0.1 x_1^n \theta^n \tag{14}$$

and

$$v x_2^{n+1} = v x_2^n + (-r_R^n) V^n$$

or

$$x_2^{n+1} = x_2^n + (0.1 x_2^n - 0.1 x_1^n)\theta^n \ . \tag{15}$$

where

v = volumetric flow rate, $ft^3/sec.$

The production of R for a definite feed condition is to be maximized by choosing optimal decisions θ^n, $n = 1, 2, \ldots, N$. This is a two-dimensional problem which not only requires a complex computational scheme but also demands a great deal of computer memory. However, the problem can be simplified by defining a new state variable

$$x_3^n = \frac{x_2^n}{x_1^n} \tag{16}$$

because of the linear transformation equations involved.

Dividing equation (15) by equation (14)

$$\frac{x_2^{n+1}}{x_1^{n+1}} = \frac{x_2^n + \theta^n(0.1x_2^n - 0.1x_1^n)}{x_1^n(1 + 0.1\theta^n)}$$

$$x_3^{n+1} = \frac{x_3^n + \theta^n(0.1x_3^n - 0.1)}{1 + 0.1\theta^n}$$

or

$$x_3^n = \frac{x_3^{n+1}(1 + 0.1\theta^n) + 0.1\theta^n}{1 + 0.1\theta^n} . \tag{17}$$

This equation gives a functional relation for determining the output ratio x_3^n at any stage in terms of the feed ratio x_3^{n+1}.

Since the production of R is to be maximized, the objective function is

$$x_2^1 - x_2^{N+1} = \sum_1^N (x_2^n - x_2^{n+1}) \tag{18}$$

and the maximum return function is

$$f_N(x_1^{N+1}, x_2^{N+1}) = \max_{\{\theta^n\}} \sum_1^N (x_2^n - x_2^{n+1}) . \tag{19}$$

Because of the linear nature of the equations, we can write

$$f_N(x_1^{N+1}, x_2^{N+1}) = x_1^{N+1} f\left(\frac{x_1^{N+1}}{x_1^{N+1}}, \frac{x_2^{N+1}}{x_1^{N+1}}\right)$$

$$= x_1^{N+1} g(x_3^{N+1}) . \tag{19}$$

Applying the dynamic programming algorithm, we have

$$f_N(x_1^{N+1}, x_2^{N+1}) = \max_{\theta^N} \left\{ (x_2^N - x_2^{N+1}) + f_{N-1}(x_1^N, x_2^N) \right\}$$

$$= \max_{\theta^N} x_1^{N+1} \left\{ \frac{x_2^N - x_2^{N+1}}{x_1^{N+1}} - \frac{x_1^N}{x_1^{N+1}} g(x_3^{N-1}) \right\} , \tag{20}$$

and the functional equation becomes

$$g_N(x_3^{N+1}) = \max_{\theta^N} \left\{ \frac{0.1\theta^N - 0.1\theta^N x_3^N}{1 + 0.1\theta^n} + \frac{1}{1 + 0.1\theta^N} g_{N-1}(x_3^N) \right\} . \tag{21}$$

Equation (21) can be solved recursively in conjunction with equation (17).

It is worth noting that there is "the menace of an expanding grid" as Bellman stated if the ratio of two state variables is greater than one. In this case, one can define an inverse ratio of two state variables which is less than one.

Therefore, one can write

$$f_N(x_1^{N+1}, x_2^{N+1}) = x_1^{N+1} g(x_3^{N+1}) = x_2^{N+1} h(x_4^{N+1}) \tag{22}$$

where

$$x_3^{N+1} = \frac{x_2^{N+1}}{x_1^{N+1}}$$

and

$$x_4^{N+1} = \frac{x_1^{N+1}}{x_2^{N+1}} .$$

In this way one can use which ever ratio is suitable, and all the functions

can be tabulated in the finite range between zero and one [12].

4. DYNAMIC PROGRAMMING WITH CONTINUOUS INDEPENDENT VARIABLE (STATE INCREMENT DYNAMIC PROGRAMMING)

A useful technique in reducing the high speed memory requirements needed to solve optimization problems by dynamic programming has been developed by Larson [13]. This new computational procedure is called dynamic programming with continuous independent variable, or state increment dynamic programming. It is based on the iterative application of Bellman's principle of optimality. It differs from the conventional method in the choice of the time interval of control. Instead of using a fixed interval, the new procedure determines the time interval as the minimum time required for at least one of the state variables to change by one increment. As a consequence of this choice of interval, the next state for any given control is known to be within a small neighborhood of the point at which control is applied. By using this result, it is possible to compute optimal control in units called blocks that cover a relatively long time interval but a small distance along each state variable. By using only one or two high speed memory locations per state in the block, it is possible to compute the optimal control throughout the block. Specialized computations near the boundaries of the block allow the optimal trajectories to pass from block to block.

This technique has been applied in a computer program which calculates minimum fuel trajectories for supersonic (Mach 3) aircraft under a variety of conditions and constraints. The basic program can be used both for a detailed evaluation of an aircraft design and for real-time control of an aircraft.

A. General problem.

Let us consider the non-autonomous system of the form

$$\frac{dx}{dt} = g(x, \theta, t) \tag{23}$$

x = s dimensional state variable

θ = r dimensional control variable

t = independent variable

g = s dimensional vector function.

Equation (23) is a set of non-linear time varying differential equations.

The system equations can be written as

$$x(t+\Delta t) = x(t) + g(x(t), \theta(t), t)\Delta t \ . \tag{24}$$

where Δt is a small incremental independent variable.

The cost function S is to be minimized by proper choice of a set of admissible control variables u.

The cost function is given as

$$S(x(t_0), \theta \ , \ t_0) = \int_{t_0}^{T} \ell(x(\tau), \theta(\tau), \tau) d\tau \tag{25}$$

t_0 = initial time

T = final time

τ = dummy variable of integration

ℓ = loss function.

B. The principle of optimality

We define

$$f(x,t) = \min_{\substack{\theta(\tau) \in U \\ t \leq \tau \leq T}} \left[\int_{t}^{T} \ell(x(\tau), \theta(\tau), \tau) d\tau\right] \tag{26}$$

The admissible control function that achieves this minimum is called the optimal control and is denoted as $\bar{\theta}(x,t)$. Invoking the principle of optimality, we write

$$f(x,t) = \min_{\{\theta\}} [\ell(x,\theta,t)\Delta t + f(x) + g(x,\theta,t)\ t,\ t + \Delta t)] \qquad (27)$$

C. The example of supersonic flight.

The notion of dynamic programming with a continuous independent variable can best be presented by considering a simple, physical example. The problem under consideration is that of calculating the optimal control of the altitude of a supersonic air transport flying at a constant velocity. The altitude h and the flight path angle α define the state and control variables respectively, and the system equation can be written as

$$\frac{dh}{dt} = g(h,\alpha,t) = v \sin\alpha \qquad (28)$$

which becomes

$$\frac{dx}{dt} = g(x,\theta,t) = v \sin\theta \qquad (29)$$

upon introduction of the above defined state and control variables.

Where v is the magnitude of the constant velocity vector, the cost function is the total fuel consumed, so that the loss function becomes

$$\ell(x,\theta,t) = \frac{dw}{dt} = W_F(x,\theta,w,t) \qquad (30)$$

where W = weight of aircraft plus fuel

W_F = fuel flow per unit time.

D. The concept of a continuous independent variable.

In the conventional dynamic programming the state variable and the independent variable, in this case time, are quantized according to the following.

The state variable, altitude, is divided into uniform increments, δh, over a finite range $0 \leq h \leq \beta$. Therefore, the state variable, x, assumes the form

$$x = j\delta h, \qquad j = 0, 1, \ldots, N \tag{31}$$

so that

$$\beta = N\delta h.$$

The independent variable is also quantized into uniform increments, δt. At every point on the h-t plane, the control variable, U, assumes values of the set of admissible controls given by

$$U = \left\{ u^{(1)}, u^{(2)}, \ldots, u^{(k)} \right\} . \tag{32}$$

In the continuous independent variable concept, the increments, δt, are not fixed but are determined by

$$\delta t = \frac{\delta h}{v \sin u} \tag{33}$$

Equation (33) then allows δt to vary over a wide range dependent upon the control variable, U.

REFERENCES

1. Nemhauser, G. L., "Introduction to Dynamic Programming," John Wiley & Sons, New York, 1966.
2. Bellman, R., "Adaptive Control Processes," Princeton Univ. Press, New Jersey, 1961.
3. Leitman, G., "Optimization Techniques," Academic Press, New York, 1962.
4. Lee, E. S., Unpublished report.
5. Roberts, S. M., "Dynamic Programming in Chemical Engineering and Process Control," Academic Press, New York, 1964.
6. Aris, R., "Discrete Dynamic Programming," Blaisdell, New York, 1964.
7. Carnahan, B., et al., "Applied Numerical Methods," Vol. 1, John Wiley & Sons, New York, 1964.
8. Aris, R., "The Optimal Design of Chemical Reactors," Academic Press, New York, 1961.
9. Kuo, M. T. and D. T. Rubin, "Optimization Study of Chemical Processes," Can. J. Chem. Eng., Vol. 40, No. 4, 152-156 (1962).
10. Kuhn, H. W. and A. W. Tucker, "Non-Linear Programming," Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability (Ed. J. Noyman), 481-492 (1950).
11. Valentine, F. A., "Contributions to the Calculus of Variations, 1933-1937) (Mathematics Dept., Univ. of Chicago), pp. 403-448, Univ. of Chicago Press, Chicago, 1937.
12. Aris, R., "Dynamic Programming," Socony Mobil Oil Co., Dallas, Texas, 1963.

13. Larson, R. E., "An Approach to Reduce the High-Speed Memory Requirement of Dynamic Programming," J. of Math. Anal. & Appl., II, 519-537 (1965).

CHAPTER V

THE K-TH BEST POLICY

It is natural that, whenever possible, the optimal policy should be used. However, it is of importance to set up the best alternative to the optimal policy for the immediate adoption in case that the optimal policy is inaccessible. Furthermore, a knowledge of the structure of the optimal and suboptimal, i.e., second best, third best,..., policies will give us a better understanding of the process. The determination of suboptimal policies also has significance in connection with sensitivity analysis in the numerical solution of an optimization problem. To solve a problem numerically, finite difference approximation is used together with digital computers. Because of the limited memory capacities of computers, we are often forced to use coarse grids of variables. Under this circumstance, a study of the neighborhood of the optimal policy can facilitate the evaluation of the meaningfulness of the solution. Thus a significant difference between the optimal and suboptimal policies may tell us that the approximation is too crude. If the suboptimal policies differ slightly from the optimal policy, we are assured that the solution is reliable.

Based on the principle of optimality, Bellman and Kalaba [1] presented an elegant method to obtain the suboptimal policies. Recently, Fan et al. [2] developed a detailed computational technique, which may be employed in applying the above-mentioned method to practical problems. In this chapter, the detailed computational technique is presented and illustrated by a simple directed network problem. An example in the optimal design of a multistage process with parallel redundancy is worked out in detail to show

how such a technique can be applied to practical problems.

1. THE ALGORITHM

For a multistage decision process (see Fig. 1 in Chapter 1) in which the state of the process stream is transformed at each stage by the decision made at that stage, a typical optimization problem is to determine the decision at each stage, subject to certain constraints, so that the objective function which is the performance criterion of the process, is maximized.

The k-th best policy is defined as the sequence of decisions which gives the objective function a value which is smaller than all those values given by 1st, 2nd,..., (k-1)-th best policies, but is at least as great as the values of the objective functions given by all other suboptimal policies, i.e. (k+1)-th, (k+2)-th,....

The algorithm given below can be used to determine the first k best policies, all at a time, for the processes with a finite difference of admissible decisions at each stage.

We define:

$\{\theta_s\}$ = the set of admissible decisions

$p_n(x,\theta_n)$ = the return function at stage n with the state of the entering stream x and the decision θ_n

$f_N = \sum_{n=1}^{N} p_n(x,\theta_n)$ = the objective function for an N-stage process

$T(x,\theta_n)$ = transformation of the state x resulting from the decision θ_n

$\underset{s}{\text{Max}}_k \{r_s\}$ = the k-th largest value of the quantities r_s, s = 1, 2,...

$f_n^{(k)}(x)$ = the value of the objective function for an n-stage process when the k-th best policy is followed and the state of the stream entering the initial stage is x.

$$f_n^{i,j} = \underset{s}{\text{Max}}_j \left\{ f_{n-1}^{(i)}(T(x,\theta_s)) + P_n(x,\theta_s) \right\}$$

To determine the optimal and suboptimal policies all at a time, we make a straightforward extension of the principle of optimality as follows [2]:

"The k-th best policy has the property that, whatever the initial state and decision are, the remaining decisions must be one of these sequences of decisions which will constitute the first k best policies with regard to the state resulting from the initial decision."

Thus, the decision at each stage in a process following the k-th best policy can be determined one by one, starting from the last stage. If we consider a certain stage at which a decision is to be made as the initial stage, it follows from the above-stated principle that only the first k best policies for the remaining part of the process need to be considered in determining the decision at the stage under consideration.

The construction of optimal tables follow the procedures stated in Section 1 of Chapter II.

Since the decision at stage n for the k-th best policy is that which gives $f_n^{(k)}(x)$, it is required to find the $f_n^{(k)}(x)$ from all possible values of the objective function. The following is a convenient way to carry it out:

(1) Compute $f_n^{i,j}$

(2) Construct the following ordered array

$$[f_n^{i,j}] = \begin{bmatrix} f_n^{1,1} & f_n^{1,2} & f_n^{1,3} & \cdots \\ f_n^{2,1} & f_n^{2,2} & f_n^{2,3} & \cdots \\ f_n^{3,1} & f_n^{3,2} & f_n^{3,3} & \cdots \\ \cdot & \cdot & \cdot\ \cdot\ \cdot\ \cdot\ \cdot & \\ \cdot & \cdot & \cdot\ \cdot\ \cdot\ \cdot\ \cdot & \\ \cdot & \cdot & \cdot\ \cdot\ \cdot\ \cdot\ \cdot & \end{bmatrix}$$

(3) $f_n^{(k)}(x)$ is then determined as the k-th largest element in $[f_n^{i,j}]$, i.e., $f_n^{(k)}(x) = \underset{i,j}{\text{Max}_k}\{f_n^{i,j}\}$. This can be conveniently carried out as follows: Let $[f_{n,k}^{i,j}]$ be the remaining ordered array obtained by eliminating from $[f_n^{i,j}]$ all those elements which constitute $f_n^{(1)}(x)$, $f_n^{(2)}(x)$,..., $f_n^{(k-1)}(x)$. Then

$$f_n^{(k)}(x) = \underset{i,j}{\text{Max}}\left\{\text{elements of } [f_{n,k}^{i,j}]\right\}$$

To determine the maximum elements in $[f_{n,k}^{i,j}]$, the first elements of each row in $[f_n^i; K^j]$ is compared until the row whose first element is $f^{i,1}$.

2. A MULTISTAGE PROCESS WITH PARALLEL REDUNDANCY

The following example shows the application of the algorithm to the optimal design of a multistage process with parallel redundancy [2]. Fig. 1 shows a multistage process in which a primary raw material is reacted with a secondary specie in the initial stage to produce an intermediate product which is then fed to the next stage and reacted with another secondary specie

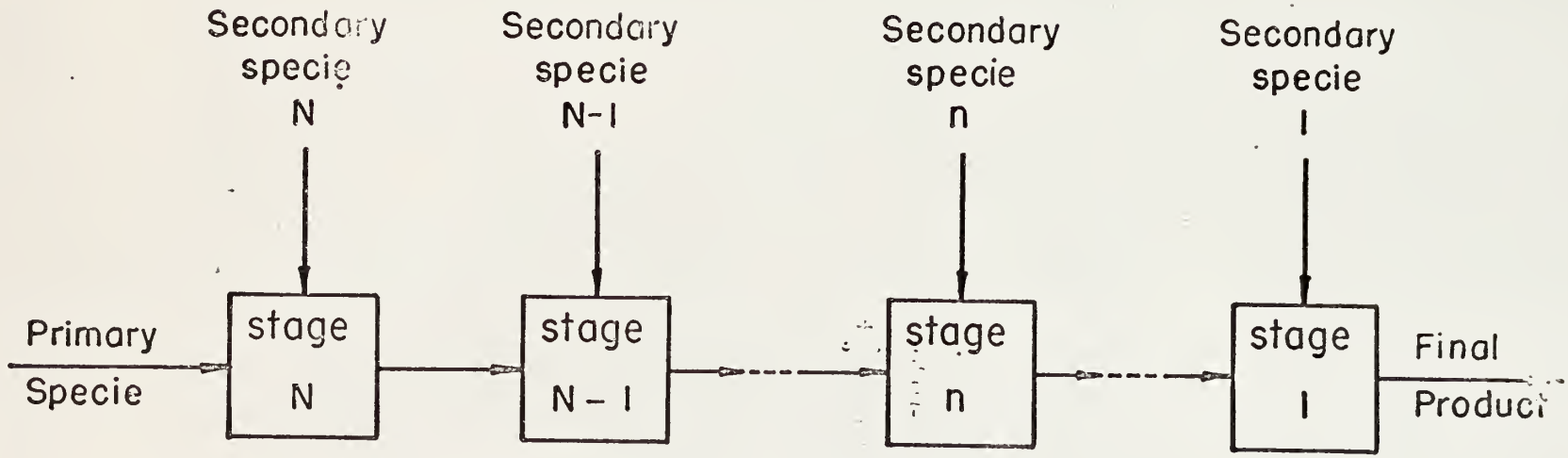


Fig. 1 Series processing sequence.

and so on through the entire process. Suppose that the secondary species are all quite unstable and cannot be stored and, therefore, must be produced upon demand by special reactions. All the intermediate products are also assumed to be unstable. Then it is clear that if a secondary specie is not available on time at any stage, the entire process will fail.

Such a failure is a stochastic phenomenon and, therefore, can be considered from a probabilistic point of view. The probability that the n-th secondary specie will be available on time is called the reliability of stage n and represented by R_n. The reliability of the whole process, R, is the probability that all the N secondary species are available on time and thus

$$R = \prod_{n=1}^{N} R_n$$

If the process which produces a certain secondary specie fails frequently, it would be desirable to produce more than one batch of that specie to increase the probability that it will be available on time. The production of more than one batch to reduce the effects of failure is named the parallel redundancy.

Suppose that b_n batches of the n-th secondary specie are prepared. Since only one batch is needed, $(b_n - 1)$ batches are reduntant. The probability that all b_n batches will fail is equal to $(1 - R_n)^{b_n}$. Hence, the probability that at least one batch will succeed is $[1 - (1 - R_n)^{b_n}]$ which is by definition the reliability of stage n with its redundancies. Thus, the reliability of the entire process with redundancy can be represented by

$$R = \prod_{n=1}^{N} [1 - (1 - R_n)^{b_n}] \qquad (1)$$

Since $b_n \geq 1$ and $R_n \leq 1$, it can be shown that

$$[1 - (1 - R_n)^{b_n}] \geq R_n$$

which indicates that the reliability of the process is increased by the use of the parallel redundancy.

Let P_g be the unit price of the final product. The expected return for the system is then expressed by $P_g R$. Let C_n be the construction cost of one reactor for the production of the n-th secondary specie (the cost is properly distributed over the life of the process), and O_n be the operating cost. Then, the net profit of the entire process, P, is

$$P = P_g R - \sum_{n=1}^{N} (C_n + O_n) b_n \qquad (2)$$

The optimal parallel redundancy is the design which maximizes P given in equation (2). Rudd [3] has applied the method of dynamic programming in the optimal design of such a process. Now let us use the algorithm described in Section 1 to find the first four best designs, all at a time.

For the sake of definiteness, we will consider a three-stage process with the following data:

	C_n	O_n	R_n for one batch
Stage 3	0.1	0.1	1/3
Stage 2	0.5	0.5	1/2
Stage 1	0.5	0.5	3/4

The unit price associated with the final product, P_g, is 10 units. Now,

if P in equation (2) is considered as the objective function, R in equation (1) as the state variable which is denoted by x, and b_n as decision, the following relations can be obtained:

$$f_1^{1,j} = \max_{b_1,j} \left\{ 10x_1 - b_1 \right\}, \qquad b_1 = 1, 2, \ldots \tag{3}$$

$$x_1 = x_2 \left[1 - \left(\frac{1}{4}\right)^{b_1} \right] \tag{4}$$

$$f_2^{i,j} = \max_{b_2,j} \left\{ f_1^i(x_2) - b_2 \right\} \qquad b_2 = 1, 2, \ldots \tag{5}$$

$$x_2 = x_3 \left[1 - \left(\frac{1}{2}\right)^{b_2} \right] \tag{6}$$

$$f_3^{i,j} = \max_{b_3,j} \left\{ f_2^i(x_3) - 0.2 \cdot b_3 \right\}, \qquad b_3 = 1, 2, \ldots \tag{7}$$

$$x_3 = x_4 \left[1 - \left(\frac{2}{3}\right)^{b_3} \right] = 1 - \left(\frac{2}{3}\right)^{b_3} \tag{8}$$

Here x_n is the reliability of the process consisting of stage n and all upstream stages. Since the primary specie is assumed to be always available, $x_4 = 1$.

For the one-stage process consisting of stage 1 only, we have

$$f_1^{(k)}(x) = f_1^{1,k}$$

This can be readily obtained and therefore the construction of the ordered array of $f_1^{i,j}$ is not necessary. A portion of the numerical results is given in Table 5.

For the two-stage process including stage 1 and stage 2, all values of $f_2^{i,j}$ are calculated from equation (5) for each possible values of x_3. The

TABLE 5

x_2	$f_1^{(1)}(x_2)$	b_1	$f_1^{(2)}(x_2)$	b_1	$f_1^{(3)}(x_2)$	b_1
0.65	4.093	2	3.875	1	3.398	3
0.70	4.562	2	4.250	1	3.890	3
0.75	5.031	2	4.625	1	4.382	3
0.80	5.500	2	5.000	1	4.875	3
0.85	5.968	2	5.375	1	5.367	3
0.90	6.437	2	5.859	3	5.750	1

TABLE 6

x_3	$f_2^{(1)}(x_3)$	b_2	x_2	i^*	$f_2^{(2)}(x_3)$	b_2	x_2	i
0.90	2.382	3	0.7875	1	2.327	2	0.6750	1
0.95	2.792	3	0.8312	1	2.679	2	0.7125	1
1.00	3.202	3	0.8750	1	3.031	2	0.7500	1

*i represents the number i in $f_{n-1}^{(i)}(T(x, \theta_n))$, which is involved in computing $f_n^{(k)}(x)$.

corresponding $f_2^{i,j}$ array is then constructed. For example, the ordered array for $x_3 = 0.9$ is

$$\begin{bmatrix} 2.382 & 2.062 & . & . & . \\ 2.327 & 1.906 & . & . & . \\ 1.909 & . & . & . & . \\ . & . & . & . & . \end{bmatrix}$$

The values of $f_2^{(k)}(x_3)$ for $x_3 = 0.9$ are then obtained from the above array. Similarly, we can find $f_2^{(k)}(x_3)$ for all other values of x_3. A part of the results is shown in Table 6.

The construction of the table for the three-stage process is similar to that for the two-stage process. However, for the three-stage process it suffices to construct only for $x_4 = 1$. The numerical results are given in Table 7. The first four highest profits for the whole process are represented by those $f_3^{(k)}(x_4)$, $k = 1, 2, 3, 4$ listed in Table 7. The corresponding optimal and suboptimal policies are then determined by the table entry technique utilizing Tables 5 through 7. For example, the optimal policy is obtained as follows:

Starting from Table 7, we find $f_3^{(1)}(x_4) = 1.322$ with $b_3 = 7$, $x_3 = 0.9414$ and $i = 1$. By means of linear interpolation, the values of b_2, x_2 and i for $x_3 = 0.9414$ can be obtained from Table 6. The results are

$$b_2 = 3 , \qquad x_2 = 0.8237 , \qquad i = 1$$

Similarly, from Table 5 we find $b_1 = 2$. The optimal and suboptimal policies thus obtained are summarized in Table 8.

TABLE 7

k	$f_3^{(k)}(x_4)$	b_3	x_3	i
1	1.322	7	0.9414	1
2	1.282	6	0.9122	1
2	1.282	8	0.9609	1
3	1.218	7	0.9414	2
4	1.212	6	0.9122	2

TABLE 8

Profit	Policies		
	b_1	b_2	b_3
1-st highest = 1.322	2	3	7
2-nd highest = 1.282	2	2	6
	2	3	8
3-rd highest = 1.218	2	2	7
4-th highest = 1.212	2	2	6

References

1. Bellman, R., and R. Kalaba, "On the K-th Best Policy," J. Soc. Indust. Appl. Math., 8, 582 (1960).

2. Fan, L. T. and C. S. Wang, "The Discrete Maximum Principle," John Wiley & Sons, New York, 1964.

3. Rudd, D. F., "Reliability Theory in Chemical System Design," I. & E. C. Fundamentals, 1, 138 (1962).

NOMENCLATURE

θ_s	the set of admissible decisions.
f_{n-1}	the optimal value of the return function for the (n-1) stages.
$f_n^{(k)}$	the value of the return function for an n-stage process in the kth best policy.
f_n	return function for an N-stage process.
P	return function of the whole process.
P_g	unit price of the final product.
$P_n(x, \theta_n)$	return of stage n with a state x and a decision θ_n.
R_n	reliability of stage n.
$T(x; \theta_n)$	transformation of the state x by the decision θ_n.

CHAPTER VI

OPTIMIZATION OF COMPLEX MULTISTAGE PROCESSES BY THE DYNAMIC PROGRAMMING TECHNIQUE

In this chapter, an application of the dynamic programming technique to the optimization of geometrically complex multistage processes is presented.

Based on the dynamic programming technique, Mitten and Nemhauser [1], and Aris [2] have presented several schemes for the optimization of certain types of geometrically complex processes. Aris, Nemhauser and Wilde [4] presented a method for formulating cyclic and branching problems. Comparative advantages and disadvantages of both methods are discussed in Ref. [5].

1. COMPLEX MULTISTAGE PROCESSES

Since a multistage process is made up by a number of stages, its features are solely determined by the types of stages of which it is composed and the way in which the stages are linked [5].

A stage is a unit consisting of at least one input and one output stream. The quantities of an input or output stream of a deterministic process are uniquely expressed by a state vector x_n and each stage is associated with a decision vector θ_n where the subscript n is the label for the stage. The state vector of the output streams from a stage is a function of the state vector of the input streams and the decision vector of that stage. As mentioned in the previous chapters, the functional relationship can be expressed in vector form as

$$x_n = T_n(x_{n-1}; \theta_n) .$$

where $T_n(x_{n-1}; \theta_n)$ is the transformation function, x_{n-1} and x_n are the input

and output state vectors of stage n respectively.

Stages can be conveniently classified according to the numbers of input and output streams associated with them. A stage with μ input streams and ν output streams will be called a (μ, ν) stage. Fig. 1 shows four basic types of stages, that is, (1,1), stage, (1,2) stage, (2,1) stage and (2,2) stage, which are also given the names of linking stage, separating stage, combining stage and complex stage, respectively [5].

A geometrically complex process can be decomposed into a primary main process and one or more than one primary side processes. The primary main process can be any combination of stages with the following properties.

(1) All of the stages are connected in series.

(2) All of the streams connecting these stages flow in the same direction.

(3) The initial stage of this combination must be one of the initial stages of the whole process, which will be called the global initial stages.

(4) The final stage of this combination must be one of the final stages of the whole process, which will be called the global final stages.

In selecting a primary main process of any process, it is desirable to include in it as many stages as possible. Stages outside the primary main process may be conveniently combined into several primary side processes. A primary side process may have one or more junctions with the primary main process. A side process connected to the main process by its final stream only will be called a parallel side process. A side process which has at least one of its initial streams linked to the main process will be called a

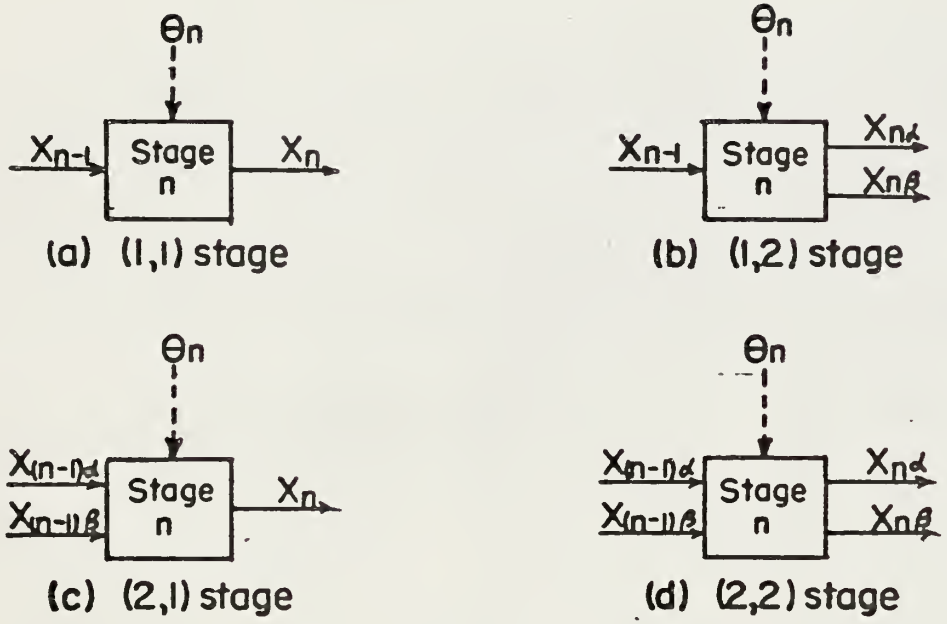


Fig. 1. Four basic types of stages.

subordinate side process or simply a subprocess.

Both the main and side processes will be denoted by the labels of their initial and final streams. For example, the complex process shown in Fig. 2 may be decomposed into a main process (0α, 9, 4β, 7), a parallel side process (0β, 9) and a subprocess (4β, 11).

It may be noted that a main process or a side process can have several initial and/or final streams. An initial stream of a main process or a side process will be called a global initial stream if it is also an initial stream of the whole process, or will be called a local initial stream if it is not an initial stream of the whole process. Similarly, a final stream will be called a global final stream if it is also a final stream of the entire process. Otherwise it is called a local final stream.

The process shown in Fig. 2 consists of two primary side processes which are themselves of the type of a simple process, that is, a process being solely composed of (1,1) stages. A primary side process may itself be geometrically a very complex process. Such a complex primary side process can be further decomposed into a secondary main process and one or several secondary side processes. A secondary main process is chosen to be a serial process. A secondary main process selected from a primary parallel side process should have a global initial stream as its initial stream and one of the local initial streams of the primary main process as its final stream. A secondary main process selected from a primary subprocess should have one of the local final streams of the primary main process as its initial stream, and a global final stream, if it has one, as its final stream. For instance, the process shown in Fig. 3 has a complex primary subprocess (2β, 10) which can be decomposed into a secondary main process (2β, 11, 9β, 10) and a

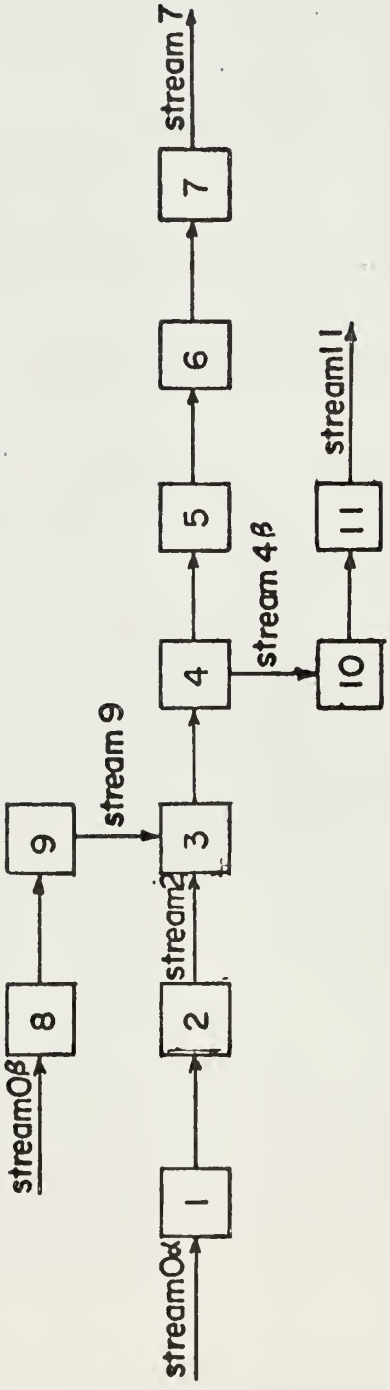


Fig. 2. A complex process with two simple side processes.

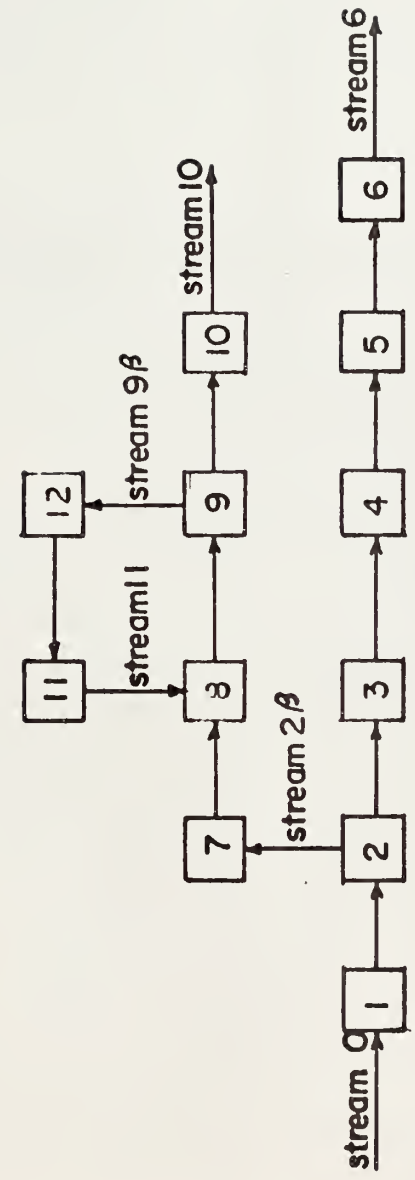


Fig. 3. A complex process with a complex side process.

secondary subprocess (9β, 11).

It is observed that any complex process can be eventually decomposed into several main processes and side processes of different ranks, all of them being serial processes [6].

2. A MULTISTAGE OPTIMIZATION PROBLEM

When a process is to be optimized, each stage is associated with a return function which is a function of the input state vectors and the decision vector. The sum of the return functions over all stages is called the objective function, that is, if the return function of stage n is $r(x_{n-1};\ \theta_n)$, the objective function of the process is $\sum_n r(x_{n-1};\ \theta_n)$. It can be seen that when all of the transformation functions are given, the objective function of the process can be expressed as a function of the global initial states and the decision vector at each stage.

The optimization problem is to find the value of the decision vector at each stage so as to maximize the objective function. All of the transformation functions are given, whereas the global initial states and final states may be either fixed or free.

Since the global initial and final states play an important role in the optimization problem, it is convenient to define a "maximum return function," (MRF) which stands for the total return of a process as a function of its global initial and final states. For example, if a process of N stages has an initial state x_0 and a final state x_N, its MRF is written as

$$f(x_0,x_N) = \max_{\theta_n} \left\{ \sum_{n=1}^{N} r(x_{n-1};\theta_n) \right\}, \qquad n = 1, 2,..., N \qquad (2)$$

with

$$\text{initial state} = x_0$$

$$\text{final state} = x_N$$

where x_0 and x_N are considered as parameters.

Once the MRF of a process has been obtained, an optimization problem with any kind of boundary conditions can be readily solved. For instance, the maximum return of a process with given initial state and free final state can be written as

$$f(\bar{\bar{x}}_0, \bar{x}_N) = \max_{x_N} f(x_0, x_N)$$

with

$$x_0 = \text{a given value}$$

where the single bar over x_N indicates that this particular value of x_N is obtained by maximizing the MRF with respect to the parameter x_N; the double bar over x_0 indicates that it is a specified value.

It is important to check the degree of freedom of an optimization problem. When both the global initial and final states are free, the degrees of freedom are equal to the sum of the global initial variables and the decision variables over all stages. When some or all of the initial and final states are specified the degree of freedom is decreased by the number of the specified state variables.

If a process has D_n decision variables at stage n, S_I global initial state variables ans S_F final state variables, then the highest degree of freedom is $(\sum_n D_n + S_I)$, and the MRF is a function of $(S_I + S_F)$ variables. It may happen that the number $(\sum_n D_n + S_I)$ is smaller than the number $(S_I + S_F)$. For such cases, the MRF can only be a function $(\sum_n D_n + S_I)$

variables; hence we must arbitrarily assign $(S_F - \sum_n D_n)$ final state variables as dependent variables. The MRF will then be written as $f(x_I, x_F \mid x_F)$, in which x_I denotes the initial state variables; x_F represents those final state variables which are considered as independent, and x_F, separated from x_I and x_F by a vertical bar, stands for those final state variables which are considered as dependent. For example, a one-stage process with $D_I = 1$, $S_I = S_F = 2$ will have its MRF written as $f(x_{0,1}, x_{0,2}, x_{1,1} \mid x_{1,2})$, in which the first subscript of x represents the label of the stream whereas the second subscript denotes the label of a component of a state vector.

3. PRINCIPLE OF OPTIMALITY AND FUNCTIONAL EQUATIONS

Since this chapter is for the purpose of extending the principle of optimality to deal with geometrically complex processes, a careful consideration of the original version of this principle will be helpful.

The principle is based on an implicit assumption that the maximum return of a process is a function of its initial state only. It is important to note that the principle of optimality was originally formulated for a simple sequential process. The final state of such a process is either specified in the problem or can be readily determined by maximizing the return of the final stage with respect to the state of the input stream of this stage, since the final state does not have any effect on other stages. Making use of this property, Bellman formulated the dynamic programming algorithm which can be represented by the following functional equation

$$f(x_{n-1}) = \underset{\theta_n}{\text{Max}} \left[r(x_{n-1}; \theta_n) + f(x_n) \right] \tag{3}$$

where x_{n-1} and x_n represent the input and output of stage n, respectively;

θ_n represents the decision of stage n; $f(x_n)$ is the MRF of the downstream subprocess (n,N), that is, the subprocess consisting of all the stages downstream to stage n, whereas $f(x_{n-1})$ is the MRF of the resulting process (n-1,N). As explained earlier, the MRF of a simple process can be expressed as a function of its initial state only.

Equation (3) can be interpreted as absorbing (imbedding) the MRF of the downstream subprocess (n,N) into the MRF of the resulting process (n-1,N). The variable x_n is an intermediate state variable of the resulting process (n-1,N) and hence must be matched when $f(x_n)$ is imbedded into $f(x_{n-1})$. The decision variable θ_n is an independent variable and must be so chosen that $f(x_{n-1})$ be maximum with respect to x_{n-1}. Thus during the process of imbedding, all the intermediate state variables must be matched, whereas all the independent variables, except those which are used as parameters for the resulting MRF, must be so chosen that the resulting MRF is maximized. When the functional equation is interpreted in this manner, its extension to dealing with a complex process will be a straightforward matter.

Now let us consider any serial process obtained from the decomposition of a complex process. If the serial process has a local final stream, the value of this local state will affect the return of its downstream subprocesses. Since such a local final state cannot be determined in the same way as that of the global final state of a simple process, it must be so chosen that the sum of the return from this serial process and the return from its downstream subprocess be maximum. A convenient way to overcome this difficulty is to express the MRF in terms of the initial and final states. Since the final state is considered as a variable, its effect on the return of its downstream subprocess can be taken into account when its value is to be fixed.

Equation (3) can then be modified to the following forms for different types of stages.

(a) for (1,1) stages,

$$f(x_{n-1}, x_F) = \underset{\theta_n}{\text{Max}} \left\{ r(x_{n-1}; \theta_n) + f(x_n, x_F) \right\} \tag{4}$$

where x_F represents the local final state

(b) for (1,2) stages,

$$f(x_{n-1}, x_{F\alpha}, x_{F\beta}) = \underset{\theta_n}{\text{Max}} \left\{ r(x_{n-1}; \theta_n) + f(x_{n\alpha}, x_{F\alpha}) + f(x_{n\beta}, x_{F\beta}) \right\} \tag{5}$$

where $x_{F\alpha}$ and $x_{F\beta}$ are the local final states of downstream subprocess $(n\alpha, F\alpha)$ and $(n\beta, F\beta)$, respectively.

(c) for (2,1) stages,

(1) if none of the input streams of stage n is one of the local final streams of the downstream subprocess:

$$f(x_{(n-1)\alpha}, x_{(n-1)\beta}, x_F) = \underset{\theta_n}{\text{Max}} \left\{ r(x_{(n-1)\alpha}; x_{(n-1)\beta}, \theta_n) + f(x_n, x_F) \right\} \tag{6}$$

(2) if one of the input streams of stage n, say stream $(n-1)\beta$, is one of the local final streams of the downstream subprocess:

$$f(x_{(n-1)\alpha}, x_F) = \underset{\theta_n, x_{(n-1)\beta}}{\text{Max}} \left\{ r(x_{(n-1)\alpha}; x_{(n-1)\beta}, \theta_n) + f(x_n, x_{(n-1)\beta}, x_F) \right\} \tag{7}$$

where the downstream subprocess is labelled by $(n, (n-1)\beta, F')$

(d) for (2,2) stages

(1) if none of the input streams of stage n is one of the local final streams of the downstream subprocess:

$$f(x_{(n-1)\alpha},x_{(n-1)\beta},x_{F\alpha},x_{F\beta}) = \max_{\theta_n} \left\{ r(x_{(n-1)\alpha};x_{(n-1)\beta},\theta_n) + f(x_{n,\alpha},x_{F\alpha}) + f(x_{n\beta},x_{F\beta}) \right\} \tag{8}$$

(2) if one of the input streams of stage n, say $x_{(n-1)\beta}$, is one of the local final streams of a downstream subprocess, say subprocess $(n\beta,(n-1)\beta,F'\beta)$

$$f(x_{(n-1)\alpha},x_{F\alpha},x_{F'\beta}) = \max_{\theta_n,x_{(n-1)\beta}} \left\{ r(x_{(n-1)\alpha};x_{(n-1)\beta},\theta_n) + f(x_{n\alpha},x_{F\alpha}) + f(x_{n\beta},x_{(n-1)\beta},x_{F'\beta}) \right\} \tag{9}$$

It can be seen that the functional equation is nothing more than absorbing (imbedding) the MRF's of the downstream subprocesses into the MRF of the process resulting from connecting the stage under consideration, the stage n, to all of its downstream stages. During the process of absorbing, the decision variable and the input states of the stage under consideration are considered as independent variables, which, except for those which are used as parameters, must be so chosen that the resulting MRF be maximum. Those initial and final states of the downstream subprocesses which become the intermediate states of the resulting process must be matched.

When the functional equation is applied to a global final-stage of the type of (1,1) stage, it becomes

(1) if the output x_n is free

$$f(x_{n-1},\bar{x}_n) = \max_{\theta_n} \left\{ r(x_{n-1};\theta_n) \right\} \tag{10}$$

(2) if the output x_n is fixed

$$f(x_{n-1},\bar{\bar{x}}_n) = \underset{\theta_n}{\text{Max}} \left\{ r(x_{n-1};\theta_n) \right\} \tag{11}$$

with $\bar{\bar{x}}$ specified.

When the functional equation is applied to local final states, it reduces to a form similar to equation (11), except that the outputs be considered as parameters. It is implicitly assumed in equations (10) and (11) that the number of the decision variables at stage n is larger than the number of its output state variables. If this is not true, the degree of freedom must be checked carefully as discussed before, and equations (10) and (11) must be changed accordingly.

Relations similar to equations (10) and (11) can also be written for the final stages which are not of the type of (1,1) stage.

4. PROCEDURES FOR OPTIMIZING COMPLEX PROCESSES

The optimal policy for a geometrically complex process may be obtained by the following procedures.

(1) Decompose the process into several main processes and side processes of different ranks as discussed in Section 1.

(2) Apply the functional equations given in the previous section to each stage to obtain the optimal decisions as functions of the initial and final states. The order of obtaining the MRF's for the side and main processes is in reverse to that of decomposing the process. In other words, the side process of the highest rank, is considered first. The MRF of a subprocess is absorbed by the main process of the same rank, and the MRF of a main process is

absorbed by the side process of the next lower rank. For example, the MRF of a secondary main process is absorbed by a primary side process. It may be noted that the MRF of a parallel side process is not absorbed by the aforementioned functional equations, but will be combined into the MRF of the main process by

$$f(x_{I\alpha},x_{I\beta},x_{F\alpha},x_{F\beta}) = \underset{x_n}{\text{Max}} \left\{ f(x_{I\alpha},x_{F\alpha},x_n) + f(x_{I\beta},x_{F\beta},x_n) \right\} \qquad (12)$$

where $(I\alpha,F\alpha,n)$ is the main process and $(I\beta,F\beta,n)$ is a parallel side process.

A parallel side process with a global initial stream as its initial stream can be converted into a subordinate side process, if it is of the type of simple process, and its transformation equation can be inverted [4]. This procedure will reduce the time of computation.

If a main or a side process has a portion which is itself of a type of simple process, the time of computation may be reduced by obtaining the MRF for this portion first and then determining its end conditions by an equation similar to equation (12). For example, the MRF for the subprocess $(0\alpha,2)$ in Fig. 2 can be obtained first and then combined with the MRF of subprocess (2, 9, 7, 11) to obtain the MRF of subprocess $(0\alpha,9,7,11)$ as

$$f(x_{0\alpha},x_9,x_7,x_{11}) = \underset{x_2}{\text{Max}} \left\{ f(x_{0\alpha},x_2) + f(x_2,x_9,x_7,x_{11}) \right\} . \qquad (13)$$

(3) Eventually we obtain the MRF of the whole process with some fixed or chosen values of the global final states, depending on whether the final states are specified in the problem or not. The initial states can then be chosen so that the total return is maximum. These values of the initial states are then used to obtain the

optimal decisions which have been expressed as functions of the global initial states. If the global initial states are specified in the problem, the decisions of the global initial states are determined by

$$f(\bar{x}_I,\bar{x}_F) = \underset{\theta_I}{\text{Max}} \left\{ r(x_I;\theta_I) + f(x_I,\bar{x}_F) \right\}$$

with

$$x_I = \bar{\bar{x}}_I = \text{a given value.}$$

EXAMPLE 1. A PROCESS WITH FEED BACK LOOPS

Let us consider the process with two staggered feedback loops shown in Fig. 4. For simplicity, we shall assume that all of the state and decision vectors are one-dimensional. The process can be decomposed into a main process (0,b,d,8β,11β,12) and two subprocesses (8β,b) and (11β,d).

The MRF of the subprocess (11β,d) can be obtained by the following equations.

$$f(x_c,x_d) = r(x_c;\theta_d) \tag{14}$$

$$f(x_{11\beta},x_d) = \underset{\theta_c}{\text{Max}} \left\{ r(x_{11\beta};\theta_c) + f(x_c,x_d) \right\} \tag{15}$$

Similarly, we may find $f(x_{8\alpha},x_{10})$, $f(x_{8\beta},x_b)$, $f(x_5,x_7)$, and $f(x_2,x_4)$. If the global final state is free, we have

$$f(x_{11\alpha},\bar{x}_{12}) = \underset{\theta_{12}}{\text{Max}} \left\{ r(x_{11\alpha};\theta_{12}) \right\} \tag{16}$$

The MRF of the whole process can then be obtained by the following equations.

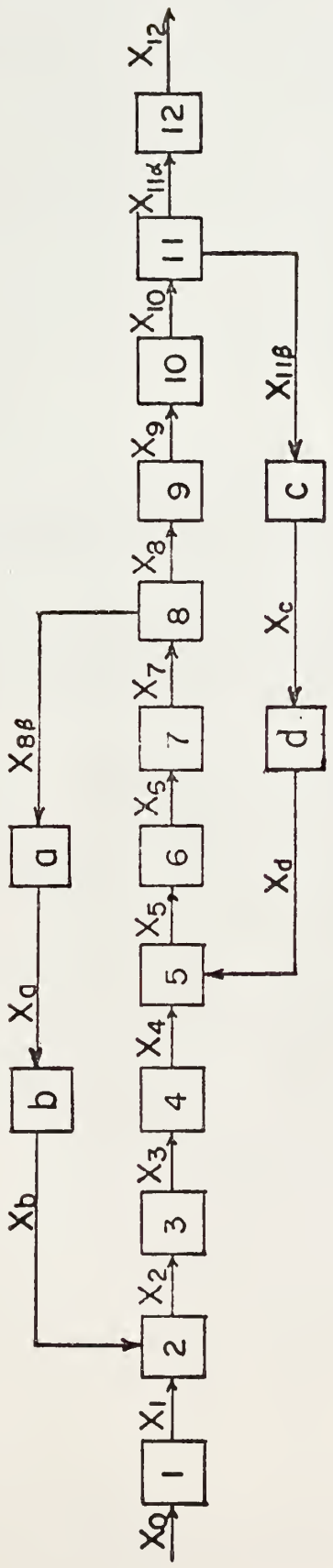


Fig. 4. A process with two staggered feedback loops.

$$f(x_{10},x_d,\bar{x}_{12}) = \underset{\theta_{11}}{\text{Max}} \left\{ r(x_{10};\theta_{11}) + f(x_{11\alpha},x_{12}) + f(x_{11\beta},x_d) \right\} \tag{17}$$

$$f(x_{8\alpha},x_d\bar{x}_{12}) = \underset{x_{10}}{\text{Max}} \left\{ f(x_{8\alpha},x_{10}) + f(x_{10},x_d,\bar{x}_{12}) \right\} \tag{18}$$

$$f(x_7,x_b,x_d,\bar{x}_{12}) = \underset{\theta_8}{\text{Max}} \left\{ r(x_7;\theta_8) + f(x_{8\beta},x_b) + f(x_{8\alpha},x_d,\bar{x}_{12}) \right\} \tag{19}$$

$$f(x_5,x_b,x_d,\bar{x}_{12}) = \underset{x_7}{\text{Max}} \left\{ f(x_5,x_7) + f(x_7,x_b,x_d,\bar{x}_{12}) \right\} \tag{20}$$

$$f(x_4,x_b,\bar{x}_{12}) = \underset{\theta_5,x_d}{\text{Max}} \left\{ r(x_4,x_d,\theta_5) + f(x_5,x_b,x_d,\bar{x}_{12}) \right\} \tag{21}$$

$$f(x_2,x_b,\bar{x}_{12}) = \underset{x_4}{\text{Max}} \left\{ f(x_2,x_4) + f(x_4,x_b,\bar{x}_{12}) \right\} \tag{22}$$

$$f(x_I,\bar{x}_{12}) = \underset{\theta_2,x_b}{\text{Max}} \left\{ r(x_I,x_b,\theta_2) + f(x_2,x_b,\bar{x}_{12}) \right\} \tag{23}$$

$$f(x_0,\bar{x}_{12}) = \underset{\theta_1}{\text{Max}} \left\{ r(x_0;\theta_I) + f(x_I,\bar{x}_{12}) \right\} \tag{24}$$

EXAMPLE 2. A STAGEWISE CROSS-CURRENT EXTRACTION PROCESS

Let us consider the cross-current extraction process with recycle as shown in Fig. 5 [8, 9]. The process consists of 3 equilibrium stages through which a solvent containing a solute passes. The solvent is fed to the system at a flow rate of q. The solute is extracted from the solvent by the addition of wash water at each stage. The solvent and wash water are assumed immiscible. A portion of the solvent from the last extractor is fed back to the first extractor at a flow rate r. Thus, the solvent flows from stage to stage at a rate, q^+r. The problem is to maximize the objective function which is the net profit per unit time by suitable choices of flow rates of wash water, w_1, w_2, and w_3.

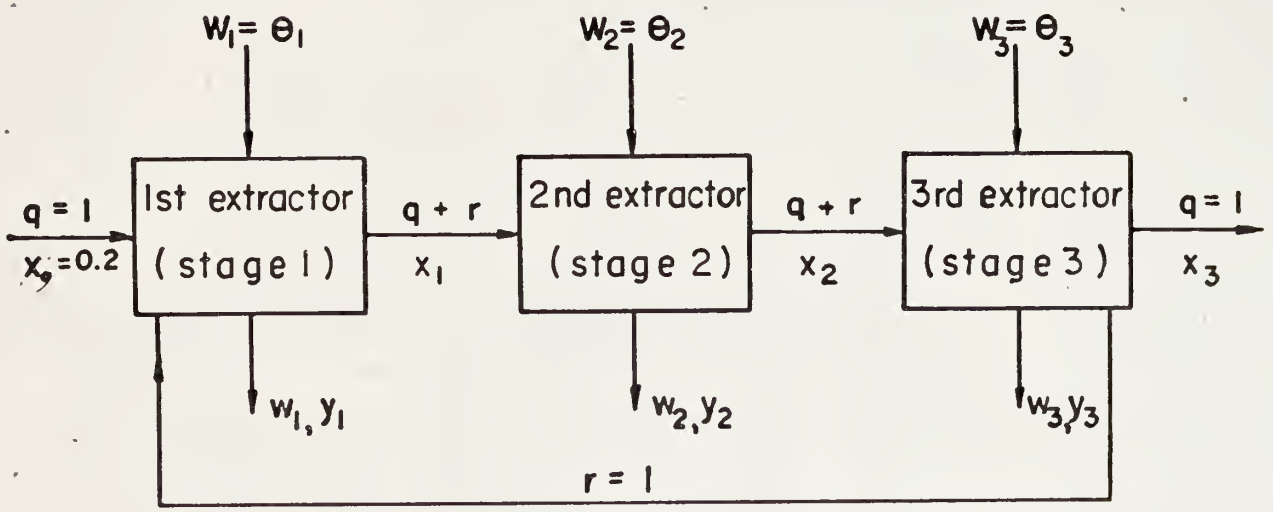


Fig.5. Schematic flow diagram for the cross-current extraction process with recycle

$$S' = \alpha q(x_0 - x_3) - \beta(w_1 + w_2 + w_3)$$

$$= \alpha\{(q+r)x_{m1} - rx_3 - qx_3\} - \beta(w_1 + w_2 + w_3)$$

$$= \alpha(q+r)(x_{m1} - x_3) - \beta(w_1 + w_2 + w_3)$$

where

$$x_{m1} = \frac{qx_0 + rx_3}{q + r}$$

and where α and β are unit prices of the solute and wash water respectively. Basing the return on the unit price of the solute, we can rewrite this as

$$S = \frac{S'}{\alpha} = q(x_0 - x_3) - \lambda(w_1 + w_2 + w_3)$$

$$= (q + r)(x_{m1} - x_3) - \lambda(w_1 + w_2 + w_3)$$

where

$$\lambda = \frac{\beta}{\alpha}$$

is the dimensionless price ratio of the wash water and solute. Note that the unit of S becomes weight per unit time according to this definition since

$$S = \frac{S'}{\alpha} = \frac{\$}{\text{time}} \times \frac{\text{lb.}}{\$} = \frac{\text{lb.}}{\text{time}}$$

The state variable is the concentration of solute x, based on the weight fraction. The decision variable at each stage is the flow rate of wash water w.

The phase equilibrium relation is given by [8],

$$y = h(x) = a + bx + cx^2 + dx^3 + ex^4 + fx^5 \qquad (25)$$

with

$a = 0.00099,$
$b = 1.7971,$
$c = 35.196,$
$d = -633.84,$
$e = 3371.3,$
$f = -5916.0.$

First we let $w_n = \theta_n$ and rewrite the objective function (or the maximum return function) as

$$\text{Max } S = f(x_0, x_3) = \underset{\{\theta_n\}}{\text{Max}} \left\{ (q + r)(x_{n-1} - x_n) - \lambda\theta_n \right\}$$

$$= \underset{\{\theta_n\}}{\text{Max}} \left\{ \sum_{n=1}^{3} r(x_{n-1}; \theta_n) \right\}$$

where $r(x_{n-1}; \theta_n)$ is the return function of stage n, which stands for the net profit per unit time at stage n based on the unit price of solute and hence it has units of weight per unit time. Applying a generalized version of the dynamic programming algorithm given in this chapter, we can write the functional equation as follows:

(1) for a one stage process including stage 3 (the third extractor) with a branching point downstream

$$f(x_2,x_3) = \underset{\theta_3}{\text{Max}} \left\{ r(x_2; \theta_3) \right\}$$

(2) for a two stage process including stage 2 (the second extractor) with a branching point downstream

$$f(x_1,x_3) = \underset{\theta_2}{\text{Max}} \left\{ r(x_1; \theta_2) + f(x_2,x_3) \right\}$$

(3) for a three stage process including all stages (all extractors) with a branching point and a combining point

$$f(x_0,x_3) = \underset{\theta_1}{\text{Max}} \left\{ r(x_0,x_3,\theta_1) + f(x_1,x_3) \right\}$$

We shall consider the case with

$$q = 1 \frac{\text{lb.}}{\text{min.}}$$

$$r = 1 \frac{\text{lb.}}{\text{min.}}$$

$$\lambda_0 = 0.05$$

$$x_6 = 0.2$$

We shall use y_n to designate the concentration of wash water flowing out of each extractor. The concentration in the fresh wash water is negligible. The return function $r(x_2; \theta_3)$ of stage 3 is

$$r(x_2; \theta_3) = (q + r)(x_2 - x_3) - \lambda\theta_3 . \tag{26}$$

From the material balance of stage 3 (the third extractor) we have

$$(q + r)(x_2 - x_3) = \theta_3 y_3 ,$$

or

$$\theta_3 = \frac{(q + r)(x_2 - x_3)}{y_3} \tag{27}$$

Substitution of equation (27) and the equilibrium relation equation (25) into equation (26), gives

$$r(x_2; \theta_3) = (q + r)(x_2 - x_3) \left\{ 1 - \frac{\lambda}{h(x_3)} \right\}$$

$$= 2(x_2 - x_3) \left\{ 1 - \frac{0.05}{h(x_3)} \right\}.$$

Similarly, the return function $r(x_1; \theta_2)$ of stage 2 (the second extractor)

is

$$r(x_1;\ \theta_2) = 2(x_1 - x_2)\quad 1 - \frac{0.05}{h(x_2)}$$

and the return function $r(x_0,x_3,\theta_1)$ of stage 1 (the first extractor) is

$$r(x_0,x_3,\theta_1) = qx_0 + rx_3 - (q + r)\, x_1 - \theta_1$$

$$= x_0 + x_3 - 2x_1 - 0.05\theta_1$$

$$= x_0 + x_3 - 2x_1 - \frac{0.05(x_0 + x_3 - 2x_1)}{h(x_1)}$$

$$= (0.2 + x_3 - 2x_1)\quad 1 - \frac{0.05}{h(x_1)}$$

RESULTS AND CONCLUSION. The computations have been performed on an I.B.M. 1620 computer. Each time, a value of the final exit concentration, x_3 is read in as a parameter as shown in the functional relations developed.

A sketch of the grid points of the state variables employed in computation and the computer flow diagram are shown in Figs. 6 and 7 respectively. The computer symbols and program are given in Tables 1 and 2.

The optimal values, the state variables and return functions obtained are as follows:

$$\bar{x}_0 = 0.1215,\quad \bar{x}_1 = 0.081,\quad \bar{x}_2 = 0.058,\quad \bar{x}_3 = 0.043$$

$$\bar{r}(x_2;\ \theta_3) = 0.01552\ \frac{\text{lb.}}{\text{min.}}\ ,$$

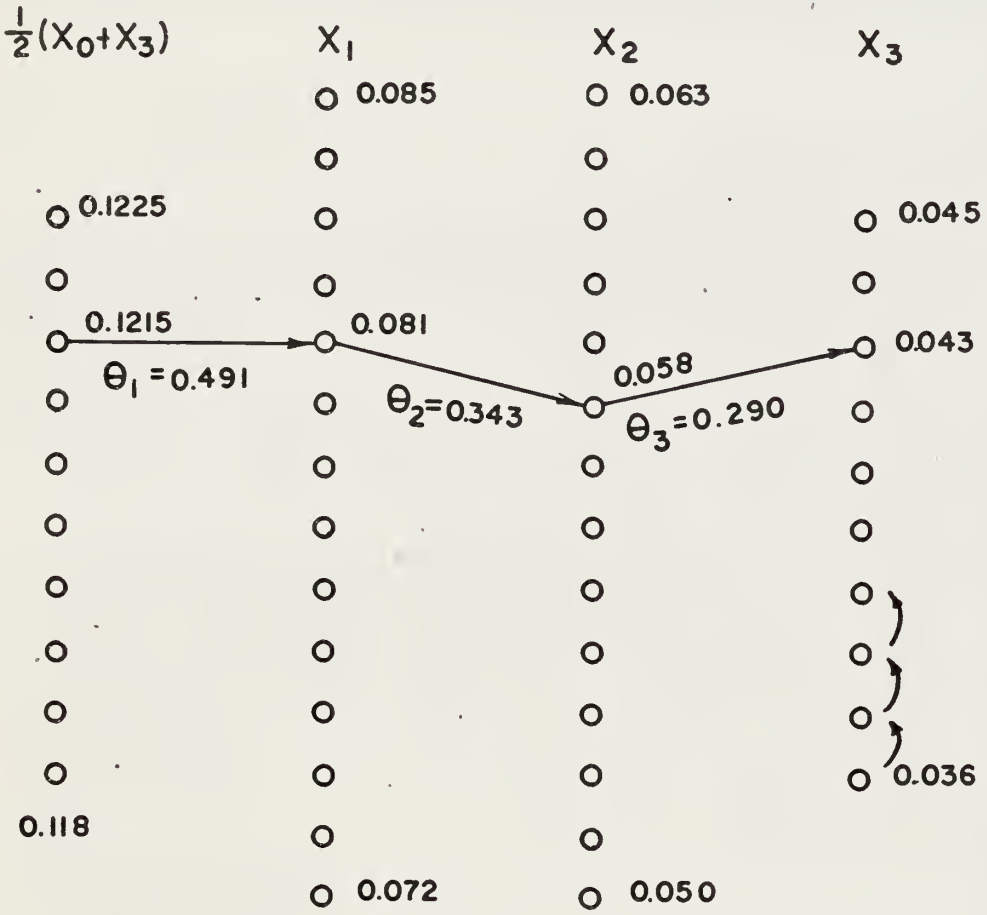


Fig. 6. A portion of the grid points taken for computation. The connected line segments show the optimal path.

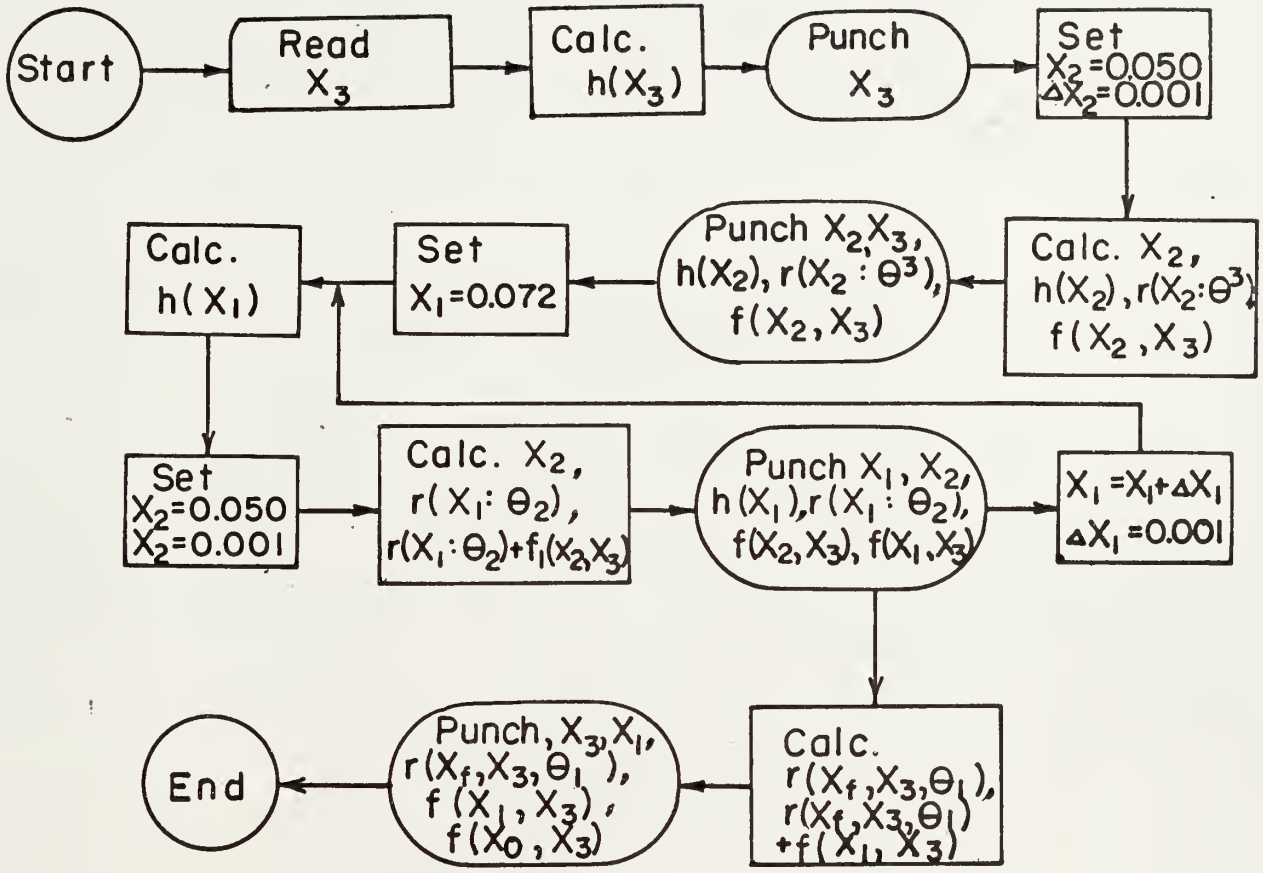


Fig. 7. Computer flow diagram for the cross-current extraction process with recycle.

TABLE 1

EXPLANATION OF PROGRAM SYMBOLS

Symbol	Explanation
X1	weight fraction of raffinate at the exit of stage 1, x_1
X2	weight fraction of raffinate at the exit of stage 2, x_2
X3	weight fraction of raffinate at the exit of stage 3, x_3
HX1	phase equilibrium function for stage 1, $h(x_1)$
HX2	phase equilibrium function for stage 2, $h(x_2)$
HX3	phase equilibrium function for stage 3, $h(x_3)$
RX2T3	return function of stage 3, $r(x_2; \theta_3)$
RX1T2	return function of stage 2, $r(x_1; \theta_2)$
RX3T1	return function of stage 1, $r(x_0, x_3, \theta_1)$
F1X2	maximum return function for a one stage process, $f(x_2, x_3)$
F2X1	maximum return function for a two stage process, $f(x_1, x_3)$
SR2F1	sum of the return function of stage 2 and the maximum return function of stage 3, $r(x_1; \theta_2) + f(x_2, x_3)$
SMRF	maximum return function for a three stage process, $f(x_0, x_3)$

TABLE 2
CROSSCURRENT EXTRACTION WITH RECYCLE

```
      DIMENSION X1(15),X2(15),HX1(15),HX2(15),RX2T3(15),F1X2(15)
      DIMENSION F2X1(15),SR2F1(15,15),SR1F2(15),RX1T2(15,15),RX3T1(15)
    1 FORMAT(6X,F8.3)
    2 FORMAT(6X,F11.5)
    3 FORMAT(6X,2F8.3,4F11.5)
      READ 1,X3
      A=.00099
      B=1.7971
      C=35.196
      D=-633.84
      E=3371.3
      F=-5916.0
      HX3=A+B*X3+C*X3**2+D*X3**3+F*X3**4+F*X3**5
      PUNCH 2,HX3
      CALC.F1X2(J)
      X2(1)=.049
      DO 11 J=2,15
      X2(J)=X2(J-1)+.001
      HX2(J)=A+B*X2(J)+C*X2(J)**2+D*X2(J)**3+E*X2(J)**4+F*X2(J)**5
      RX2T3(J)=2.*(X2(J)-X3)*(1.-.05/HX3)
      F1X2(J)=RX2T3(J)
      PUNCH 3,X2(J),X3,HX2(J),RX2T3(J),F1X2(J)
   11 CONTINUE
      CALC.F2X1(K)
      X1(1)=.071
      DO 16 K=2,15
      X1(K)=X1(K-1)+.001
      HX1(K)=A+B*X1(K)+C*X1(K)**2+D*X1(K)**3+E*X1(K)**4+F*X1(K)**5
      DO 17 J=2,15
      RX1T2(K,J)=2.*(X1(K)-X2(J))*(1.-.05/HX2(J))
      SR2F1(K,J)=RX1T2(K,J)+F1X2(J)
      IF(J-2)18,18,19
   18 F2X1(K)=SR2F1(K,J)
   19 IF(SR2F1(K,J)-F2X1(K))17,17,20
   20 F2X1(K)=SR2F1(K,J)
      PUNCH 3,X1(K),X2(J),HX1(K),RX1T2(K,J),F1X2(J),F2X1(K)
   17 CONTINUE
   16 CONTINUE
      CALC.SMRF
      DO 21 K=2,15
      RX3T1(K)=(.2+X3-2.*X1(K))*(1.-.05/HX1(K))
      SR1F2(K)=RX3T1(K)+F2X1(K)
      IF(K-2)22,22,23
   22 SMRF=SR1F2(K)
   23 IF(SR1F2(K)-SMRF)21,21,24
   24 SMRF=SR1F2(K)
      PUNCH 3,X3,X1(K),RX3T1(K),F2X1(K),SMRF
   21 CONTINUE
      END
```

$$\bar{r}(x_1;\ \theta_2) = 0.02886\ \frac{\text{lb.}}{\text{min.}}\ ,$$

$$\bar{r}(x_0,\ x_3,\ \theta_1) = 0.05647\ \frac{\text{lb.}}{\text{min.}}\ ,$$

$$f(x_2,\ x_3) = 0.01552\ \frac{\text{lb.}}{\text{min.}}$$

$$f(x_1,\ x_3) = 0.04439\ \frac{\text{lb.}}{\text{min.}}$$

$$f(x_0,\ x_3) = 0.10086\ \frac{\text{lb.}}{\text{min.}}$$

The optimal value of the decision variable at the first extractor is

$$\bar{\theta}_1 = \frac{\bar{r}(x_0,\ x_3,\ \theta_1)}{h(\bar{x}_1) - \lambda}$$

$$= \frac{0.05647}{0.16512 - 0.05}$$

$$= 0.491\ \frac{\text{lb.}}{\text{min.}}$$

Similarly, we have

$$\bar{\theta}_2 = 0.343\ \frac{\text{lb.}}{\text{min.}}$$

and

$$\bar{\theta}_3 = 0.290\ \frac{\text{lb.}}{\text{min.}}$$

It must be understood that there are small errors in these results due to discretization.

We see that the allocation of wash water is in the decreasing order as indicated in Refs. [9] and [5]. The small differences among the optimal values obtained from this problem and those given in Refs. [9] and [5] are due to the slight differences in phase equilibrium relationship and the

differences in the errors due to the discretization. The optimal values of θ_n and the maximum return functions of Refs. [9] and [5], and from this study are given in Table 3.

The optimal results and the best results corresponding to each final exit concentration x_3 are listed in Table 4. Some non-optimal results are also shown in Table 5 for comparison. It is clear that the profit based on unit price of the solute in each non-optimal case is smaller than the optimal value of 0.10086 $\frac{\text{lb.}}{\text{min.}}$ corresponding to the value of x_3 at 0.043, as given in Table 3.

TABLE 3

COMPARISON OF OPTIMAL VALUES

Case — Optimal values	θ_1 lb. min.	θ_2 lb. min.	θ_3 lb. min.	RMF lb. min.
Ref. 9	0.518	0.335	0.274	0.1018
Ref. 5	0.610	0.440	0.420	0.0974
this study	0.491	0.343	0.290	0.1009

TABLE 4

COMPARISON OF OPTIMAL RESULTS FOR VARIOUS VALUES OF EXIT CONCENTRATION, x_3

$x_{m1} = \frac{x_0+x_3}{2}$ wt. fraction	x_1 wt. fraction	x_2 wt. fraction	x_3 wt. fraction	$f(x_2,x_3)$ $\times 10^2$ lb./min.	$f(x_1,x_3)$ $\times 10^2$ lb./min.	$f(x_0,x_3)$ $\times 10^2$ lb./min.	θ_1 lb./min.	θ_2 lb./min.	θ_3 lb./min.
0.1180	0.075	0.051	0.036	1.276	4.091	9.986	0.541	0.397	0.347
0.1185	0.076	0.052	0.037	1.323	4.170	10.016	0.531	0.391	0.336
0.1190	0.076	0.053	0.038	1.368	4.126	10.040	0.538	0.368	0.326
0.1195	0.077	0.054	0.039	1.409	4.195	10.058	0.528	0.363	0.318
0.1200	0.078	0.055	0.040	1.448	4.261	10.072	0.519	0.357	0.310
0.1205	0.079	0.056	0.041	1.485	4.323	10.081	0.510	0.352	0.303
0.1210	0.080	0.057	0.042	1.519	4.383	10.085	0.500	0.348	0.296
0.1215*	0.081*	0.058*	0.043*	1.552*	4.439*	10.086*	0.491*	0.343*	0.290*
0.1220	0.082	0.059	0.044	1.583	4.492	10.082	0.481	0.338	0.284
0.1225	0.082	0.060	0.045	1.612	4.415	10.045	0.487	0.319	0.278

*Optimal results

TABLE 5

NON-OPTIMAL RESULTS

$x_{m1} = \frac{x_1+x_3}{2}$ wt. fraction	θ_1 lb./min.	$r(x_0,x_3,\theta_1)$ lb./min.	x_1 wt. fraction	θ_2 lb./min.	$r(x_1;\theta_2)$ lb./min.	x_2 wt. fraction	θ_3 lb./min.	$r(x_2;\theta_3)$ lb./min.	x_3 wt. fraction	Total $Sx10^2$ lb./min.
0.1210	0.530	0.05949	0.078	0.336	0.02715	0.056	0.276	0.01418	0.042	10.083
0.1220	0.512	0.05842	0.080	0.328	0.02761	0.058	0.265	1.01478	0.044	10.081
0.1190	0.521	0.06149	0.074	0.381	0.02697	0.051	0.283	0.01185	0.038	10.035
0.1225	0.549	0.06157	0.078	0.298	0.02510	0.058	0.241	0.01391	0.045	10.064

References:

1. Mitten, L. G., and G. L. Nemhauser, "Multistage Optimization," Chem. Engg. Prog., 59, No. 1, 52 (1963).

2. Nemhauser, G. L., "Introduction to Dynamic Programming," John Wiley & Sons, New York, 1966.

3. Aris, R., "Discrete Dynamic Programming," Blaisdell Publishing Co., New York, 1964.

4. Aris, R., G. L. Nemhauser, and D. Wilde, "Optimization of Cyclic and Branching Systems by Serial Procedures," A.I.Ch.E. Journal, 10, 913 (1964).

5. Fan, L. T., and C. S. Wang, "The Discrete Maximum Principle," John Wiley, New York, 1964.

6. Fan, L. T., "The Continuous Maximum Principle," John Wiley & Sons, New York, 1966.

7. Bellman, R., "Dynamic Programming," Princeton Univ. Press, New Jersey, 1957.

8. Lee, E. S., "Optimization by a Gradient Technique," I.E.C. Fundamentals, Vol. 3, No. 4, Nov. 1964.

9. Rosen, E. M., "Further Comments on the Paper, 'Optimum Cross Current Extraction with Product Recycle.'"

APPENDICES

APPENDIX I

ANALYSIS, DESIGN, AND SIMULATION OF A MULTIEFFECT, MULTISTAGE EVAPORATOR SYSTEM

Water administrators throughout the world are greatly concerned about supplementing water supplies as the demands for fresh water increase year by year. For many years, fresh water has been obtained from salt water by flash evaporation due to the comparative lower cost of converting sea water into potable water by means of large capacity flash evaporators. More water is needed than can be provided by the natural sources of supply and it seems likely that the desalination of sea water is turning out to be a must. As a consequence, much recent effort has been directed to the development of desalting plants with the purpose of producing large quantities of fresh water at low costs. It is anticipated that multieffect multistage (MEMS) flash evaporator systems can economically provide fresh water to areas with large population. This study is essentially concerned with the design and simulation of a multieffect multistage flash evaporation system with a nominal capacity of 50 MM (50 million) gallons per day. The process model is similar to that of the proposed pilot plant at Millstone (1).

The outstanding feature of this process which distinguishes it from other flash evaporation processes is that a portion of the flashing brine stream from each effect is recycled back to the inlet of that effect. This scheme is more efficient thermodynamically than recycling the spent brine from the last effect directly to the first effect. The recycle stream is passed through condenser tube bundles on which water vapor is condensing in order to preheat the recycle brine prior to mixing it with the brine stream coming from the previous effect. Since heat recovery becomes more efficient as the number of

stages used for flashing and preheating increases, inter-effect recycling makes it possible to add more stages per temperature gradient as pressure difference increases.

There are many design variables to consider and many ways to carry out the simulation. The number of stages, total temperature difference (temperature difference between the flashing and recycle brine), blowdown temperature or concentration at the outlet of each effect, allocation of number of stages in each effect, and selection of brine velocities are all important, but the most important factors are the first two. In this simulation study, we chose a 68 stage model with 23 stages in the first and the second effects and 22 stages in the third effect.

Two models of the system a "micro stage model" and a "macro stage model" are used. In the micro stage model the performance of each stage within the heat recovery section of each effect is considered, while in the macro stage model the performance of each heat recovery section is considered as a unit. In both models, we treat each heat rejection section as a unit even though we assume that there are 3 stages in the heat rejection section of the first and second effects and 2 stages in the third. Since each heat rejection section also acts as a brine heater for the next effect, it is much more convenient to treat them as a whole unit. In both models, we assume equal distillate production for each effect (this automatically fixes the blowdown concentration of each effect). In the former, we examine the effect of changing the total temperature difference and the blowdown temperature for each effect, while in the latter we fix the blowdown temperature and study the effect of changing the total temperature difference.

1. PROCESS DESCRIPTION

Assume that the MEMS plant is located on the coast about 50 feet above the sea level. The sea water is usually pumped from the ocean via forebays or sumps. It passes through the heat rejection section of the third effect and its pH value is adjusted by adding sulfuric acid. Then it goes to the deaerator system where the dissolved oxygen and nitrogen (inert gases) and a small amount of carbon dioxide are removed. The pretreated raw feed is heated by passage through the condenser tubes of the heat recovery section of the third effect and all of the stages of the second and the first effects. It is finally heated to the desired flashing temperature by a shell and tube brine heater with low pressure steam from an adjacent power plant. Before entering the flashing chamber of the first effect, the heated feed is mixed with the recycle brine from the outlet of the same effect. The recycle brine is heated to the same temperature as the heated feed by passing it through the brine heater also. Under these circumstances, the mixing streams are at the same temperature and the concentration differences are reduced because the whole system has been divided into three effects. The free energy decreases due to mixing, that is, the thermodynamic irreversibility has thus been reduced. The flashing brine then cascades from stage to stage as a result of the pressure differential maintained. In each stage, a portion of the water flashes from the brine solution. It is condensed on the condenser tubes via demisters and is caught in troughs. The distillate also cascades from stage to stage and is finally pumped to the storage tanks as product from the lowest pressure end, i.e., the last stage of the third effect. The brine in excess of that required for recycle in the third effect is pumped out of the system and discharged to the ocean as a blowdown. A schematic diagram of the process is shown in Figs. 1 and 2.

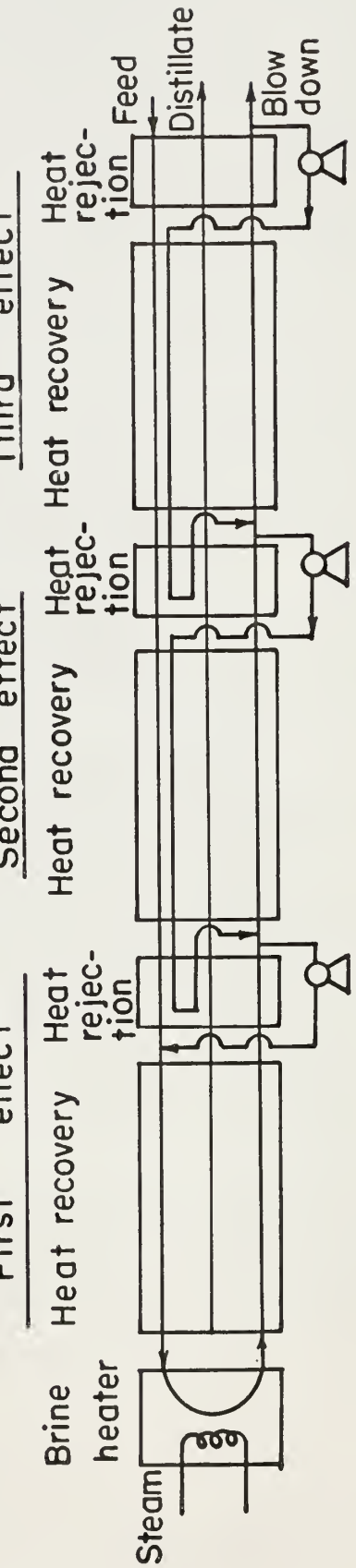


Fig. 1. Process flow diagram of the multieffect multistage flash evaporator system.

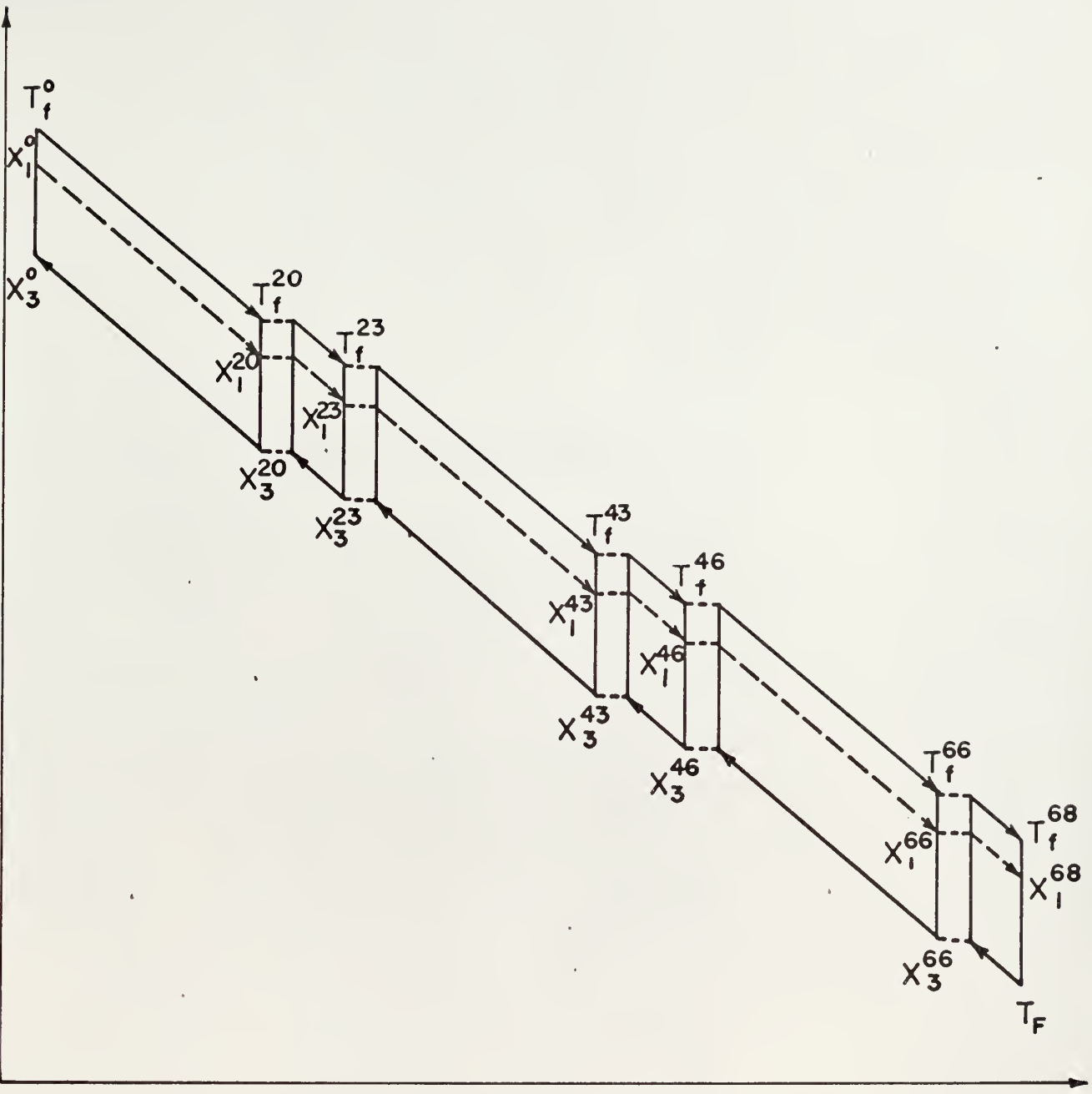


Fig. 2. Temperature profiles of the multi-effect multi-stage flash evaporator system (The micro stage model).

2. FORMULATION OF THE DESIGN EQUATIONS ACCORDING TO THE MICROSTAGE MODEL

By making an analysis of the process, the design equations for the simulation study may be developed. In this simulation study a 68 stage, 50 million gallons per day plant is investigated. It is assumed that the salt water fed to the system contains 3.5 weight per cent salt and that the concentrated brine leaving the system (blowdown) contains 7 weight per cent salt. This information is presented together with other numerical data in Table 7.

(A) Material and Energy Balances for the nth Stage of the Heat Recovery Section of the First Effect. From Fig. 3, we may develop the following material and energy balance relationships. A distillate material balance gives*

$$x_2^n = x_2^{n-1} + \Delta W^n \,, \tag{1}$$

where ΔW^n depends on the energy balance

$$\left\{F(1+r_1) - x_2^{n-1}\right\}(C_p^{n-1})_{f1}\, T_f^{n-1} = \Delta W^n H_v^n + \left\{F(1+r_1) - x_2^n\right\}(C_p^n)_{f1}\, T_f^n \,, \tag{2}$$

where

T_f = temperature of flashing brine (^oF),

ΔW = amount of water vapor formed (lb/hr),

H_v = enthalpy of water vapor relative to liquid to 0^o F (BTU/lb),

$(C_p)_{f1}$ = heat capacity of flashing brine (BTU/lb^oF),

r_1 = ratio of the recycle brine in the first effect to the make-up feed (lb/lb),

x_2 = amount of distillate (lb/hr).

---

*All superscripts denote stage numbers. A complete list of nomenclature is given in Table 2 on page 200.

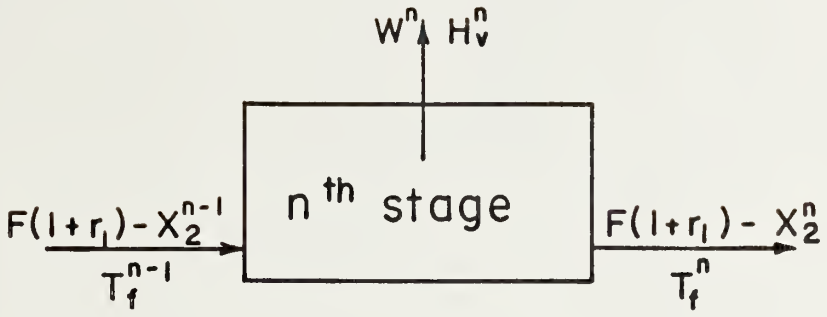


Fig. 3. Block diagram for the flashing brine at the n-th stage, heat recovery section of the first effect.

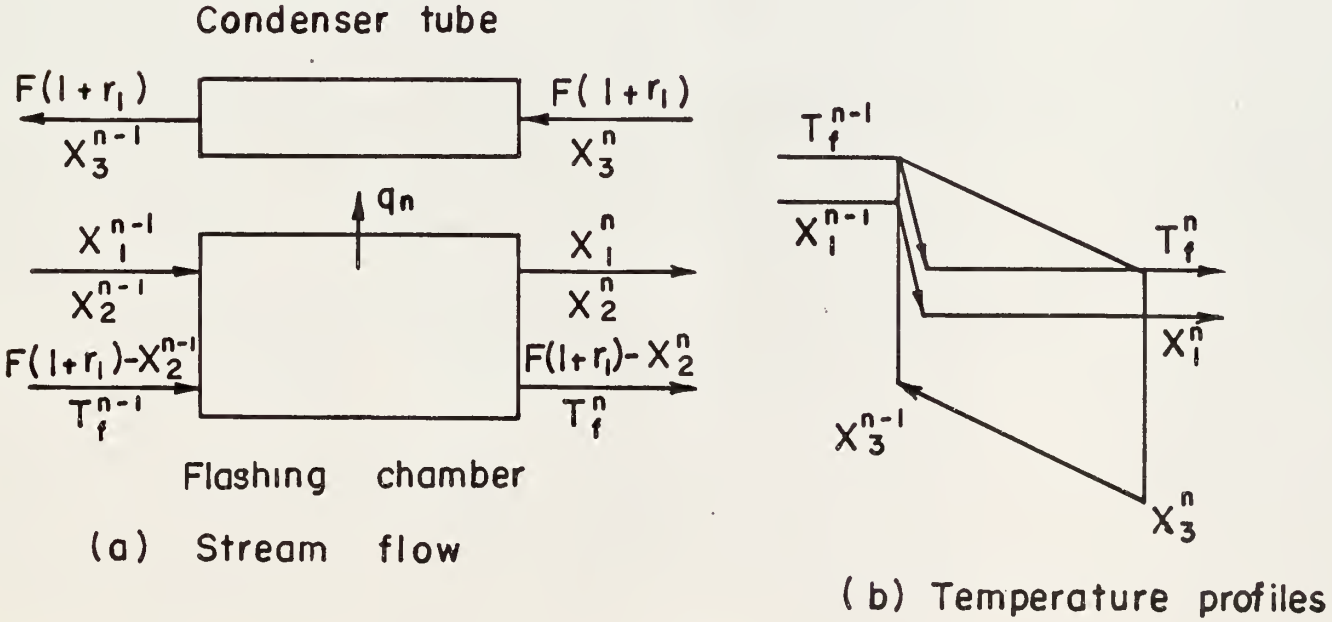


Fig. 4. Block diagram for the operation of the n-th stage, heat recovery section of the first effect.

Equation (2) can be simplified if we put

$$(C_p^{n-1})_{fl} = (C_p^n)_{fl} = (C_p)_{fl} = \text{average heat capacity of the flashing brine in the first effect (BTU/lb}^{\circ}\text{F)}$$

Then we have,

$$(C_p)_{fl} = \frac{\frac{(C_p)_F + r_1(C_p^{23})_{fl}}{1+r_1} + (C_p^{23})_{fl}}{2} = \frac{(C_p)_F + (1+2r_1)(C_p^{23})_{fl}}{2(1+r_1)}$$

where

$(C_p)_F$ = heat capacity of the make-up feed (BTU/lb$^{\circ}$F),

$(C_p^{23})_{fl}$ = heat capacity of the flashing brine at stage 23 (BTU/lb$^{\circ}$F).

According to the Bechtel Corporation (3), heat capacities of brine at various concentrations can be expressed as

$$C_p = 1-c \tag{3}$$

in which c is the concentration of the brine in weight fraction. The enthalpy of water vapor can be written as

$$H_v^n = (C_p)_W x_1^n + \lambda^n \tag{4}$$

where

$(C_p)_W$ = 1.0 = heat capacity of distillate (BTU/lb$^{\circ}$F),

x_1 = temperature of distillate ($^{\circ}$F),

λ^n = latent heat of vaporization (BTU/lb).

Thus, equation (2) becomes

$$\{F(1+r_1) - x_2^{n-1}\}(C_p)_{f1}\, T_f^{n-1} = \Delta W^n(x_1^n + \lambda^n) + \{F(1+r_1) - x_2^{n-1} - \Delta W^n\}$$

$$(C_p)_{f1}\, T_f^n \qquad (5)$$

Solving for ΔW^n gives

$$\Delta W^n = \frac{F(1+r_1) - x_2^{n-1}\,(C_p)_{f1}(T_f^{n-1} - T_f^n)}{\lambda^n + (x_1^n - (C_p)_{f1} T_f^n)} \qquad (6)$$

Substituting equation (6) into equation (1), we have (see Fig. 4)

$$x_2^n = x_2^{n-1} + \frac{\{F(1+r_1) - x_2^{n-1}\}(C_p)_{f1}(T_f^{n-1} - T_f^n)}{\lambda^n + (x_1^n - (C_p)_{f1}\, T_f^n)} . \qquad (7)$$

The temperature of the distillate in each stage x_1^n depends upon the pressure that is maintained in that stage. The temperature difference

$$\theta^n = x_1^{n-1} - x_1^n \qquad (8)$$

depends on the difference in pressure that is maintained. Noting that

$$T_f^{n-1} = x_1^{n-1} + \Delta t_{BPE}^{n-1} ,$$

$$T_f^n = x_1^n + \Delta t_{BPE}^n ,$$

we have

$$T_f^{n-1} - T_f^n = \theta^n + \Delta t_{BPE}^{n-1} - \Delta t_{BPE}^n .$$

According to reference (3), the boiling point elevation of the flashing brine at each stage is approximately equal to 2^oF. Thus, we put

$$\Delta t_{BPE}^{n-1} = \Delta t_{BPE}^n = 2.$$

Furthermore, since the term $x_1^n - (C_p)_{f1} T_f^n$ is negligibly small compared with λ^n, equation (7) can be simplified further to obtain

$$x_2^n = x_2^{n-1} + \frac{\{F(1+r_1) - x_2^{n-1}\}(C_p)_{f1}\,\theta^n}{\lambda^n} \qquad (9)$$

with $x_2^0 = 0.$

An energy balance for the flash chamber of the nth stage gives

$$q^n = x_2^{n-1}(C_p)_W x_1^{n-1} + \{F(1+r_1) - x_2^{n-1}\}(C_p)_{f1} T_f^{n-1}$$

$$- x_2^n(C_p)_W x_1^n - \{F(1+r_1) - x_2^n\}(C_p)_{f1} T_f^n ,$$

or

$$q^n = x_2^{n-1} x_1^{n-1} + \{F(1+r_1) - x_2^{n-1}\}(C_p)_{f1}(x_1^{n-1} + \Delta t_{BPE}^{n-1})$$

$$- (x_2^{n-1} + \Delta W^n)(x_1^{n-1} - \theta^n)$$

$$- \{F(1+r_1) - x_2^{n-1} - \Delta W^n\}(C_p)_{f1}(x_1^{n-1} - \theta^n + \Delta t_{BPE}^n),$$

The above expression may be further simplified to give

$$q^n = x_2^{n-1}\,\theta^n + \{F(1+r_1) - x_2^{n-1}\}(C_p)_{f1}(\theta^n + \Delta t_{BPE}^{n-1} - \Delta t_{BPE}^n)$$

$$+ \Delta W^n \left((C_p)_{f1}(x_1^n + \Delta t_{BPE}^n) - x_1^n\right)$$

Since

$$\Delta t_{BPE}^{n-1} = \Delta t_{BPE}^n$$

and the last term is negligibly small, we can write

$$q^n = x_2^{n-1}\,\theta^n + \{F(1+r_1) - x_2^{n-1}\}\,(C_p)_{f1}\,\theta^n \,. \qquad (10)$$

For the fluid inside the condenser tubes we have the following energy balance

$$q^n = F(1+r_1)\,(C_p)_{r1}\,(x_3^{n-1} - x_3^n) \qquad (11)$$

with

$$x_3^0 = T_f^o - \Delta t_1$$

where x_3 = temperature of recycle brine (^oF),

T_f^o = maximum brine temperature (^oF),

Δt_1 = temperature rise by passage through the brine heater (^oF),

$(C_p)_{r1}$ = heat capacity of recycle brine (BTU/lb^oF).

$(C_p)_{r1}$ is calculated as

$$(C_p)_{r1} = \frac{(C_p)_F + r_1 (C_p^{23})_{f1}}{1 + r_1} \,.$$

The condenser tube area needed for each stage may be determined from the equation

$$q^n = U^n A^n (\Delta t^n)_{L.M.T.D.} \qquad (12)$$

where

U^n = overall heat transfer coefficient at stage n (BTU/ft^{2}hr),

$(\Delta t^n)_{L.M.T.D.}$ = logarithmic mean temperature difference for heat transfer at stage n(^oF),

$$(\Delta t^n)_{L.M.T.D.} = \frac{(x_1^n - x_3^n) - (x_1^n - x_3^{n-1})}{\ell n \dfrac{x_1^n - x_3^n}{x_1^n - x_3^{n-1}}} = \frac{x_3^{n-1} - x_3^n}{\ell n \dfrac{x_1^n - x_3^n}{x_1^n - x_3^{n-1}}} \qquad (13)$$

Combining equations (10) and (11), we have

$$x_3^n = x_3^{n-1} - \frac{\theta^n \left[F(1+r_1)(C_p)_{f1} + x_2^{n-1}(1 - (C_p)_{f1})\right]}{F(1+r_1)(C_p)_{r1}} \qquad (14)$$

From equations (8), (11), (12) and (13), we can obtain

$$A^n = \frac{q^n}{U^n \dfrac{q^n}{F(1+r_1)(C_p)_{r1} \ell n \dfrac{x_1^n - x_3^n}{x_1^n - x_3^{n-1}}}} = \frac{F(1+r_1)(C_p)_{r1}}{U^n} \ell n \frac{x_1^n - x_3^n}{x_1^n - x_3^{n-1}}$$

$$= \frac{F(1+r_1)(C_p)_{r1}}{U^n} \left[\ell n\ (x_1^{n-1} - \theta^n - x_3^n) - \ell n\ (x_1^{n-1} - \theta^n - x_3^{n-1})\right] \qquad (15)$$

Taking $U^n = (U_1)_{av}$ as the average overall heat transfer coefficient for the condenser tubes in the first effect, and combining equations (14) and (15), we obtain

$$A^n = \frac{F(1+r_1)(C_p)_{r1}}{(U_1)_{av}} \left[\ell n \left\{x_1^{n-1} - \theta^n - x_3^{n-1} + \frac{\theta^n \left\{F(1+r_1)(C_p)_{f1} + x_2^{n-1}(1-(C_p)_{f1})\right\}}{F(1+r_1)(C_p)_{r1}}\right\}\right.$$

$$\left. - \ell n\ (x_1^{n-1} - \theta^n - x_3^{n-1})\right], \quad n = 1, 2, \ldots, 20 \qquad (16)$$

(B) Cost Equations for the Brine Heater and the Heat Recovery Section of the First Effect. In the following, we shall consider the unit production cost in dollars per pound of distillate term by term. The total production is $\frac{F}{2}$ so that each cost item is divided by F/2 to give the unit production cost in dollars per pound of distillate.

(a) Steam cost. The amount of steam consumed, S is

$$S = \frac{F(1+r_1)(C_p)_{r1}\Delta t_1}{\lambda_s}$$

The steam cost in dollars per pound of distillate produced, $(x_4)_s$ is

$$(x_4)_s = \frac{C_1 F(1+r_1)(C_p)_{r1}\Delta t_1}{\frac{F}{2}\lambda_s} = \frac{2C_1(1+r_1)(C_p)_{r1}\Delta t_1}{\lambda_s} \qquad (17)$$

where

λ_s = latent heat of steam (BTU/lb)

C_1 = unit steam cost ($/lb)*

(b) Fixed charge cost for the brine heater. The amount of heat transferred in the brine heater, q_B, is

$$q_B = F(1+r_1)(C_p)_{r1}\Delta t_1 = U_B A_B \Delta t_{L.M.T.D.}$$

where

---

*All unit cost items are from (3).

$$\Delta t_{L.M.T.D.} = \frac{(T_s - 250 + \Delta t_1) - (T_s - 250)}{\ell n \frac{T_s - 250 + \Delta t_1}{T_s - 250}} = \frac{\Delta t_1}{\ell n \frac{T_s - 250 + \Delta t_1}{T_s - 250}}$$

T_s = temperature of the steam.

In case steam of 40 psi is used, $T_s = 274.4^{\circ}F$ and

$$\Delta t_{L.M.T.D.} = \frac{\Delta t_1}{\ell n \frac{24.4 + \Delta t_1}{24.4}}$$

Using the above equations, the heat transfer area in the brine heater, A_B, becomes

$$A_B = \frac{F(1+r_1)(C_p)_{rl}\Delta t_1}{U_B \frac{\Delta t_1}{\ell n \frac{24.4+\Delta t_1}{24.4}}} = \frac{F(1+r_1)(C_p)_{rl}}{U_B} \{\ell n(24.4+\Delta t_1) - \ell n(24.4)\}$$

and the fixed charge cost for the brine heater per pound of distillate produced, $(x_4)_B$, is written as

$$(x_4)_B = \frac{C_2 F(1+r_1)(C_p)_{rl}}{\frac{F}{2} U_B} \{\ell n(24.4 + \Delta t_1) - \ell n(24.4)\}$$

or

$$(x_4)_B = \frac{2C_2(1+r_1)(C_p)_{rl}}{U_B} \{\ell n(24.4 + \Delta t_1) - \ell n(24.4)\} \qquad (18)$$

where C_2 is the unit fixed charge cost for the brine heater ($/ft^2 hr).

(c) Fixed charge cost for the condenser tubes.

From equation (16), the fixed charge cost for the condenser tubes per

pound of distillate product, $(x_4^n)_{c1}$, becomes

$$(x_4^n)_{c1} = \frac{C_3 F(1+r_1)(C_p)_{r1}}{\frac{F}{2}(U_1)_{av}} \left(\ell n \left(x_1^{n-1} - \theta^n - x_3^{n-1} + \frac{\theta^n}{F(1+r_1)(C_p)_{r1}} \times \{ F(1+r_1)(C_p)_{f1} \right.\right.$$

$$\left.\left. + x_2^{n-1}(1-(C_p)_{f1}) \} \right) - \ell n \left(x_1^{n-1} - \theta^n - x_3^{n-1} \right) \right)$$

$$(x_4^n)_{c1} = \frac{2C_3(1+r_1)(C_p)_{r1}}{(U_1)_{av}} \left(\ell n \left(x_1^{n-1} - \theta^n - x_3^{n-1} + \frac{\theta^n}{F(1+r_1)(C_p)_{r1}} \times \{ F(1+r_1)(C_p)_{f1} \right.\right.$$

$$\left.\left. + x_2^{n-1}(1-(C_p)_{f1}) \} \right) - \ell n \left(x_1^{n-1} - \theta^n - x_3^{n-1} \right) \right) \qquad (19)$$

where C_3 is the unit fixed charge cost for the condenser tubes ($\$/ft^2$ hr).

(d) Cost of recycle for the first effect. The cost of recycle which we wish to consider results because of the pressure differences created in order to produce flashing at each stage. In order to recycle some of the brine which leaves stage 23, we must increase its pressure to that of the brine stream flowing from the brine heater to the first stage. The work that must be done to accomplish this, W_{r_1}, is

$$W_{r_1} = Fr_1 \times \frac{\Delta P_1}{\rho} \times \frac{144}{3600 \times 550} \text{ HP-hr.}$$

where

ρ = density of the flashing brine = 62.5 (lb/ft^3)

$\Delta P_1 = P_0 - P_1$,

P_0 = vapor pressure of brine entering stage one at T_f^o (psi),

The vapor pressure of the brine leaving stage 23, P_1, is calculated by an empirical formula [4], that is,

$$P_1 = \exp\left(14.07 - \frac{9 \times 3660}{5(x_3^{20} - 32) + 1989}\right) \quad \text{(psi)}$$

We can write the cost of recycle, $(x_4)_{r1}$ as

$$(x_4)_{r1} = \frac{C_4 \, Fr_1(P_0 - P_1) \times 144}{\frac{F}{2} \times 62.5 \times 550 \times 3600 \times 0.85} = \frac{2C_4 r_1(P_0 - P_1) \times 144}{62.5 \times 550 \times 3600 \times 0.85} \qquad (20)$$

where C_4 is the unit pumping cost including the electric power and depreciation cost for the pumps and the correction factor 0.85, which accounts for the efficiency of the pumps, is taken from reference (3).

For the heat recovery section of the first effect, the accumulated cost per pound of distillate produced, x_4^n, is*

$$x_4^n = (x_4)_s + (x_4)_B + (x_4^n)_{cl}, \qquad n = 1, 2, \ldots, 20$$

or

$$x_4^n = (x_4)_s + (x_4)_B + \frac{2C_3(1+r_1)(C_p)_{rl}}{(U_1)_{av}} \left\{ \ell n \left[x_1^{n-1} - \theta^n - x_3^{n-1} + \frac{\theta^n}{F(1+r_1)(C_p)_{rl}} \right.\right.$$

$$\left.\left. \{F(1+r_1)(C_p)_{fl} + x_2^{n-1}(1 - (C_p)_{fl})\} \right] - \ell n(x_1^{n-1} - \theta^n - x_3^{n-1}) \right\} \qquad (21)$$

$$n = 1, \ldots, 20.$$

(C) Material and Energy Balances and Cost Equations for the Heat Rejection Section of the First Effect. The heat rejection section of the first effect also acts as the brine heater for the second effect. In this study, the

---

*The cost of recycle for the first effect will be included when the cost of the heat rejection section of the first effect is considered.

temperature of the brine leaving the flash chamber of the last stage of the heat rejection section is assumed to be equal to the temperature of the feed stream which enters the heat recovery section, that is,

$$x_3^{20} = T_f^{23} = x_1^{23} + 2$$

An energy balance around the heat rejection section of the first effect gives (see Fig. 5)

$$F(1+r_1)(C_p)_{f1}(x_1^{20} + \Delta t_{BPE}^2 - x_3^{20}) = \{F(C_p)_F + Fr_2(C_p^{46})_{f2}\}(x_3^{20} - x_3^{23})$$

According to reference (3)

$$(C_p)_F = 0.965$$

and $$(C_p^{46})_{f2} = 1 - 0.035 \times \frac{3}{2} = 1 - 0.0525 = 0.9475$$

Solving for x_3^{23}, we have

$$x_3^{23} = x_3^{20} - \frac{(1+r_1)(C_p)_{f1}(x_1^{20} + 2 - x_3^{20})}{0.965 + r_2 \times 0.9475} \qquad (22)$$

The amount of distillate produced in the heat rejection section of the first effect is given by

$$(\Delta W)_{1j} = \frac{\{F(1+r_1) - x_2^{20}\}(C_p)_{f1}(T_f^{20} - T_f^{23})}{(\lambda)_{avlj}}$$

or

$$(\Delta W)_{1j} = \frac{[F(1+r_1) - x_2^{20}](C_p)_{f1}(x_1^{20} + 2 - x_3^{20})}{1098.3 - 0.3055(x_1^{20} + x_3^{20} + 2)} \qquad (23)$$

where the formula for λ is obtained by curve fitting the steam table

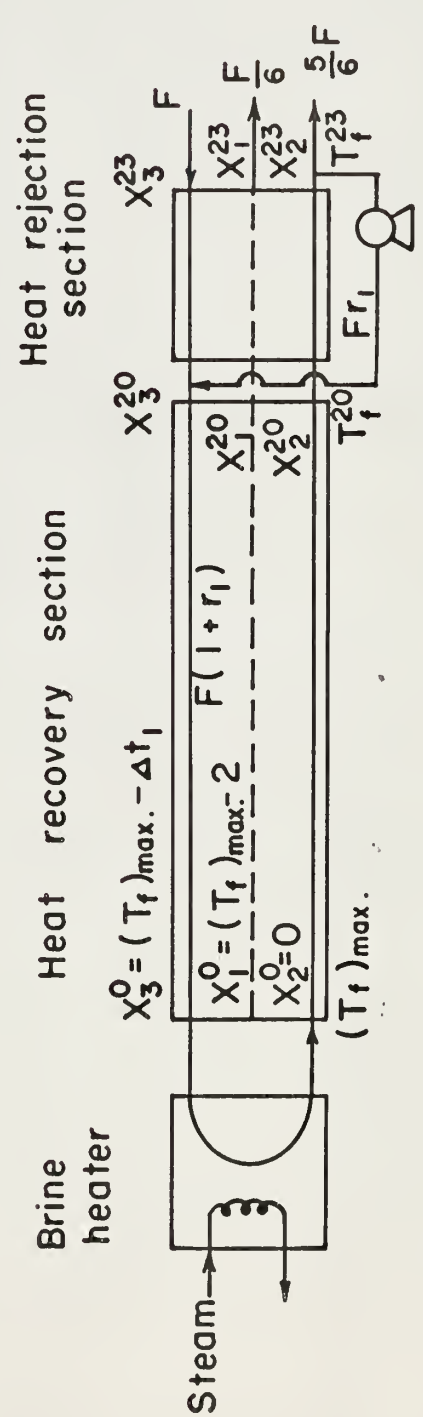


Fig. 5. Schemetic flow diagram for the first effect.

$$\lambda = 1098.3 - 0.611\, x_1$$

Thus

$$(\lambda)_{avlj} = \frac{1098.3 - 0.611(x_1^{20} + 2) + 1098.3 - 0.611\, x_3^{20}}{2}$$

$$= 1098.3 - 0.3055(x_1^{20} + 2 + x_3^{20})$$

The heat transfer area required for the condenser tubes of the heat rejection section of the first effect is

$$A_{1j} = \frac{q_{1j}}{(U_1)_{av}(\Delta t)_{avlj}} = \frac{F(1+r_1)(C_p)_{f1}(x_1^{20} + 2 - x_3^{20})}{(U_1)_{av}\,(\Delta t)_{avlj}} \qquad (24)$$

where $(\Delta t)_{avlj}$ is evaluated as follows

$$\Delta t_{avlj} = \frac{(x_1^{21} - x_3^{20}) + (x_1^{23} - x_3^{23})}{2}$$

From Fig. 7-a, we see that

$$x_1^{21} = x_1^{20} - \frac{x_1^{20} + 2 - x_3^{20}}{3}$$

Using the above equation together with the assumption that

$$x_1^{23} = x_3^{20} - 2$$

we obtain

$$\Delta t_{avlj} = \frac{3(x_3^{20} - x_3^{23}) + 2(x_1^{20} - x_3^{20}) - 8}{6} \qquad (25)$$

Substitution of equation (25) into equation (24) yields

$$A_{1j} = \frac{6\,F(1+r_1)(C_p)_{f1}(x_1^{20} + 2 - x_3^{20})}{(U_1)_{av}\{3(x_3^{20} - x_3^{23}) + 2(x_1^{20} - x_3^{20}) - 8\}}$$

Hence, the unit production cost is obtained as

$$(x_4)_{1j} = \frac{6\,FC_3(1+r_1)(C_p)_{f1}(x_1^{20} + 2 - x_3^{20})}{\frac{F}{2}(U_1)_{av}\{3(x_3^{20} - x_3^{23} + 2(x_1^{20} - x_3^{20}) - 8\}}$$

$$= \frac{12C_3(1+r_1)(C_p)_{f1}(x_1^{20} + 2 - x_3^{20})}{(U_1)_{av}\{3(x_3^{20} - x_3^{23}) + 2(x_1^{20} - x_3^{20}) - 8\}} \qquad (26)$$

(D) Material and Energy Balances and Cost Equations for the Heat Recovery Section of the Second Effect. Using Fig. 6, we can carry out an analysis for the heat recovery section of the second effect. Equations analogous to those obtained for the first effect can be derived. The temperature of distillate, x_1^n, may still be determined from equation (8), that is,

$$x_1^n = x_1^{n-1} - \theta^n, \qquad n = 24,\ldots, 43 \qquad (27)$$

with

$$x_1^{23} = x_3^{20} - 2$$

where we take Δt_{BPE} as 2^oF.

The amount of distillate can be determined from

$$x_2^n = x_2^{n-1} + \frac{\{F(\frac{5}{6} + r_2) - x_2^{n-1}\}(C_p)_{f2}\,\theta^n}{\lambda^n}, \qquad n = 24,\ldots, 43 \qquad (28)$$

with

$$x_2^{23} = 0 .$$

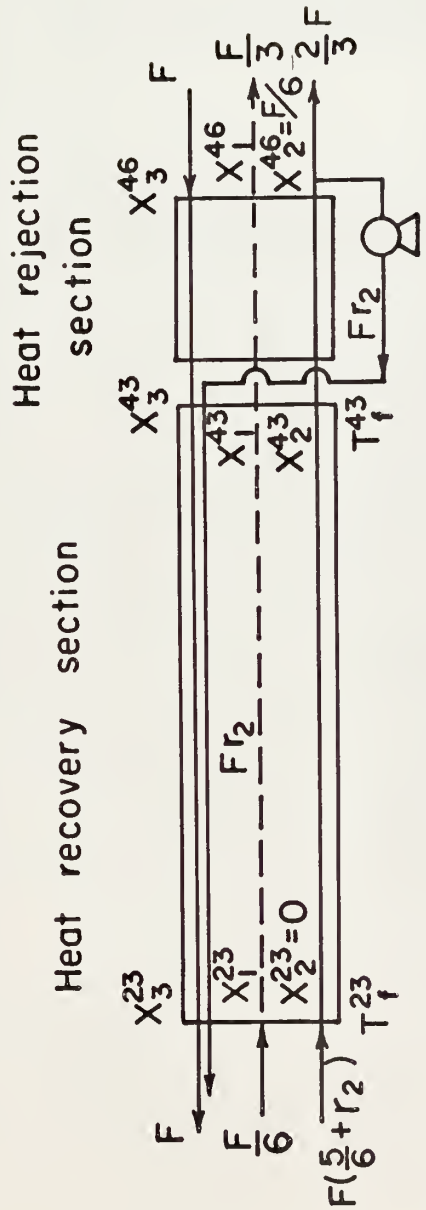
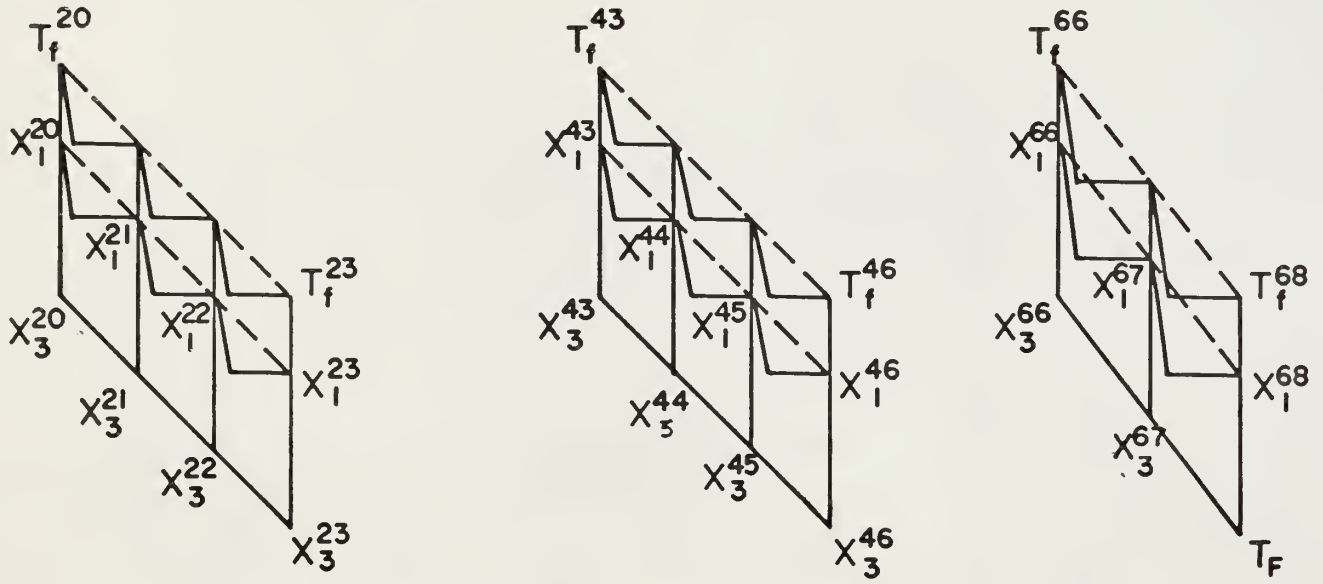


Fig. 6. Schemetic flow diagram for the second effect.



(a) The first effect (b) The second effect (c) The third effect

Fig. 7. Temperature differences for heat transfer in the heat rejection section of each effect.

which is analogous to equation (9) for the first effect expect that F is replaced by $\frac{5}{6}$ F as $\frac{1}{6}$ of the make-up feed has been flahsed out in the previous effect. It should also be noted that the amount of distillate refers only to the distillate formed after entering the second effect. As a matter of fact, the distillate produced in the first effect just gives up its sensible heat when it cascades down the subsequent effects, and it does not affect the quantity of water that is flashed from the brine.

By using a procedure similar to that used to obtain equation (14), we can obtain the recursive equation for x_3 as

$$x_3^n = x_3^{n-1} - \frac{\{F(\frac{5}{6} + r_2)(C_p)_{f2} + x_2^{n-1}(1-(C_p)_{f2}) + \frac{F}{6}\}\theta^n}{F(0.965 + r_2 \times 0.9475)} \qquad (29)$$

$$n = 24, \ldots, 43.$$

Similarly, the heat transfer area for the condenser tubes that is required at each stage may be obtained by analogy. The equation which corresponds to equation (16) for the first effect is

$$A^n = \frac{F(0.965 + r_2 \times 0.9475)}{(U_2)_{av}} \times \left(\ln(x_1^{n-1}-\theta^n-x_3^n)-\ln(x_1^{n-1}-\theta^n-x_3^{n-1})\right)$$

$$= \frac{F(0.965 + r_2 \times 0.9475)}{(U_2)_{av}} \times \left(\ln\left[x_1^{n-1}-\theta^n-x_3^{n-1}\right.\right.$$

$$\left.\left. + \frac{\{F(\frac{5}{6} + r_2)(C_p)_{f2} + x_2^{n-1}(1-(C_p)_{f2}) + \frac{5}{6}\}\theta^n}{F(0.965 + r_2 \times 0.9475)}\right] - \ln(x_1^{n-1}-\theta^n-x_3^{n-1})\right) \qquad (30)$$

$$n = 24, \ldots, 43$$

Multiplication of A^n by $\frac{2C_3}{F}$ gives the fixed charge cost. The recycle cost is obtained by using exactly the same procedure as that used for the first

effect. We obtain

$$(x_4)_{r2} = \frac{2 \times C_4 \times r_2 \times 144(P_1-P_2)}{62.5 \times 550 \times 3600 \times 0.85} \tag{31}$$

where

$$P_2 = \exp\ 14.07 - \frac{9 \times 3660}{5(x_3^{43} - 32) + 1989}$$

Thus, the unit production cost x_4^n becomes

$$x_4^n = x_4^{23} + \frac{2C_3(0.965 + r_2 \times 0.9475)}{(U_2)_{av}} \left(\ln\left[x_1^{n-1}-\theta^n-x_3^{n-1} + \frac{\left\{F(\frac{5}{6}+r_2)(C_p)_{f2}+x_2^{n-1}(1-(C_p)_{f2} + \frac{5}{6}\right\}\theta^n}{F(0.965 + r_2 \times 0.9475)}\right] - \ln(x_1^{n-1}-\theta^n-x_3^{n-1})\right)$$

$$n = 24,\ldots, 43\ , \tag{32}$$

where

$$x_4^{23} = x_4^{20} + (x_4)_{1j} + (x_4)_{r1}\ .$$

which are the accumulated cost up through stage 20, the cost of the condenser tube area for the heat rejection section of the first effect, and the cost of recycle in the first effect, respectively.

(E) Material and Energy Balances and Cost Equations for the Heat Rejection Section of the Second Effect. The heat rejection section of the second effect also acts as the brine heater for the third effect. As before, we assume that the operation is such that

$$x_3^{43} = T_f^{46} = x_1^{46} + 2$$

An energy balance for the heat rejection section of the second effect gives

$$F(\frac{5}{6} + r_2)(C_p)_{f2}(T_f^{43}-T_f^{46}) + \frac{F}{6}(x_1^{43}-x_1^{46}) = \{F(C_p)_F + Fr_3(C_p^{68})_{f3}\}(x_3^{43}-x_3^{46})$$

The following approximate form of this equation will be used here.

$$F(1+r_2)(C_p)_{f2}(x_1^{43} + 2 - x_3^{43}) = \{F(C_p)_F + Fr_3(C_p^{68})_{f3}\}(x_3^{43}-x_3^{46})$$

According to (3)

$$(C_p)_F = 0.965$$

and

$$(C_p^{68})_{f3} = 0.930.$$

Solving for x_3^{46}, we have

$$x_3^{46} = x_3^{43} - \frac{(1+r_2)(C_p)_{f2}(x_1^{43} + 2 - x_3^{43})}{0.965 + r_3 \times 0.93} . \qquad (33)$$

The production of distillate in the heat rejection section of the second effect may be calculated as follows:

$$(\Delta W)_{2j} = \frac{\{F(\frac{5}{6} + r_2) - x_2^{43}\}(C_p)_{f2}(T_f^{43} - T_f^{46})}{(\lambda)_{av2j}}$$

Since

$$(\lambda)_{av2j} = 1098.3 - 0.3055(x_1^{43} + 2 + x_3^{43})$$

we obtain

$$(\Delta W)_{2j} = \frac{\{F(\frac{5}{6} + r_2) - x_2^{43}\}(C_p)_{f2}(x_1^{43} + 2 - x_3^{43})}{1098.3 - 0.3055(x_1^{43} + 2 + x_3^{43})} \qquad (34)$$

The heat transfer area required for the condenser tubes of the heat rejection section of the second effect is

$$A_{2j} = \frac{q_{2j}}{(U_2)_{av}(\Delta t)_{av2j}} = \frac{F(1+r_2)(C_p)_{f2}(x_1^{43} + 2 - x_3^{43})}{(U_2)_{av}(\Delta t)_{av2j}} \tag{35}$$

where (see Fig. 7b)

$$(\Delta t)_{av2j} = \frac{3(x_3^{43} - x_3^{46}) + 2(x_1^{43} - x_3^{43}) - 8}{6} \tag{36}$$

Substitution of equation (36) into equation (35) yields

$$A_{2j} = \frac{6F(1+r_2)(C_p)_{f2}(x_1^{43} + 2 - x_3^{43})}{(U_2)_{av}\{3(x_3^{43}-x_3^{46})+2(x_1^{43}-x_3^{43})-8\}}$$

Hence, the unit production cost will be

$$(x_4)_{2j} = \frac{12C_3(1+r_2)(C_p)_{f2}(x_1^{43} + 2 - x_3^{43})}{(U_2)_{av}\{3(x_3^{43} - x_3^{46}) + 2(x_1^{43} - x_3^{43}) - 8\}} . \tag{37}$$

(F) Material and Energy Balances and Cost Equations for the Heat Recovery Section of the Third Effect. Using Fig. 8 and an analysis which is analogous to that used in Sections (A) and (D), equations which describe the heat recovery section of the third effect can be obtained. Equation (8) for the temperature of the distillate may still be used, that is,

$$x_1^n = x_1^{n-1} - \theta^n, \qquad n = 47,\ldots,66 \tag{38}$$

where

$$x_1^{46} = x_3^{43} - 2.0$$

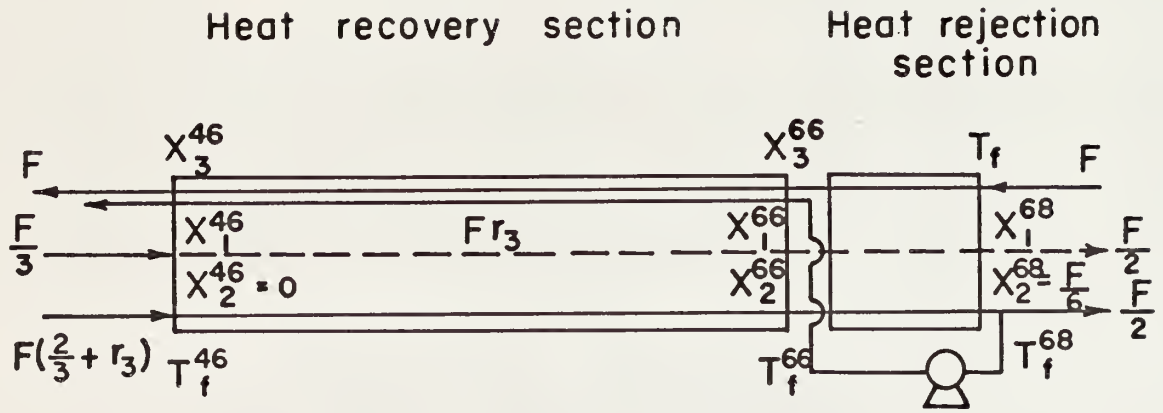


Fig. 8. Schemetic flow diagram for the third effect.

The amount of distillate can be determined from

$$x_2^n = x_2^{n-1} + \frac{\{F(\frac{2}{3} + r_3) - x_2^{n-1}\}(C_p)_{f3}\,\theta^n}{\lambda^n}, \qquad n = 47,\ldots, 66, \quad (39)$$

with $x_2^{46} = 0.$

which is analogous to equation (9) for the first effect except that F is replaced by $\frac{2}{3}$ F as $\frac{1}{3}$ of the make-up feed has been flahsed in the previous two effects. Again, note that the amount of distillate refers only to the new distillate which is obtained after entry of the flashing brine to the third effect.

By using a procedure similar to that used to obtain equations (14) and (26), we can obtain

$$x_3^n = x_3^{n-1} - \frac{\{F(\frac{2}{3} + r_3)(C_p)_{f3} + x_2^{n-1}(1-(C_p)_{f3}) + \frac{F}{3}\}\,\theta^n}{F(0.965 + r_3 \times 0.930)}, \qquad (40)$$

$$n = 47,\ldots, 66,$$

with x_3^{46} calculated from equation (33).

The heat transfer area, A^n, may be obtained by using a procedure like that used to obtain equation (16). It is given by

$$A^n = \frac{F(0.965+r_3 x 0.93)}{(U_3)_{av}} \left(\ln(x_1^{n-1}-\theta^n-x_3^n) - \ln(x_1^{n-1}-\theta^n-x_3^{n-1})\right)$$

$$= \frac{F(0.965+r_3 x 0.93)}{(U_3)_{av}} \left(\ln\{x_1^{n-1}-\theta^n-x_3^{n-1}\right.$$

$$\left. + \frac{\{F(\frac{2}{3} + r_3)(C_p)_{f3} + x_2^{n-1}(1-(C_p)_{f3}) + \frac{F}{3}\}\theta^n}{F(0.965 + r_3 \times 0.93)}\right)$$

$$\left. - \ln(x_1^{n-1} - \theta^n - x_3^{n-1})\right), \qquad n = 47,\ldots, 66, \qquad (41)$$

Multiplication of A^n by $\frac{2C_3}{F}$ gives the fixed charge cost. The recycle cost is obtained by using exactly the same procedure as that used for the first effect. We obtain

$$(x_4)_{r3} = \frac{2 \times C_4 \times r_3 \times 144 \times (P_2 - P_3)}{62.5 \times 550 \times 3600 \times 0.85} . \qquad (42)$$

Where

$$P_3 = \exp\left(14.07 - \frac{9 \times 3660}{5(x_3^{66} - 32) + 1989}\right) \text{ in } (\text{lb/in}^2).$$

We are now able to write the accumulated unit production cost as

$$x_4^n = x_4^{46} + \frac{2C_3(0.965 + r_3 \times 0.93)}{(U_3)_{av}} \left[\ln(x_1^{n-1} - \theta^n - x_3^n) - \ln(x_1^{n-1} - \theta^n - x_3^{n-1})\right], \quad n = 47, \ldots, 66 \qquad (43)$$

where

$$x_4^{46} = x_4^{43} + (x_4)_{2j} + (x_4)_{r2}$$

which are the accumulated cost up through stage 43, the cost of the condenser tube area for the heat rejection section of the second effect, and the cost of recycle in the second effect, respectively.

(G) Material and Energy Balances and Cost Equations for the Heat Rejection Section of the Third Effect. We again assume that the operation is such that

$$x_3^{66} = T_f^{68} = x_1^{68} + 2$$

An energy balance for the heat rejection section of the third effect gives

$$q_{3j} = F(\frac{2}{3} + r_3)(C_p)_{f3}(T_f^{66} - T_f^{68}) + \frac{F}{3}(x_1^{66} - x_1^{68})$$

The following approximate form of this equation will be used.

$$q_{3j} \doteq F(1+r_3)(C_p)_{f3}(x_1^{66} + 2 - x_3^{66})$$

The production of distillate in the heat rejection section of the third effect may be calculated from the equations

$$(\Delta W)_{3j} = \frac{\{F(\frac{2}{3} + r_3) - x_2^{66}\}(C_p)_{f3}(T_f^{66} - T_f^{68})}{(\lambda)_{av3j}}$$

Since

$$(\lambda)_{av3j} = 1098.3 - 0.3055\ (x_1^{66} + 2 + x_3^{66})$$

we can obtain

$$(\Delta W)_{3j} = \frac{\{F(\frac{2}{3} + r_3) - x_2^{66}\}(C_p)_{f3}(x_1^{66} + 2 - x_3^{66})}{1098.3 - 0.3055(x_1^{66} + 2 + x_3^{66})} \qquad (44)$$

The heat transfer area required by the condenser tubes of the heat rejection section of the third effect is

$$A_{3j} = \frac{q_{3j}}{(U_3)_{av}(\Delta t)_{av3j}} = \frac{F(1+r_3)(C_p)_{f3}(x_1^{66} + 2 - x_3^{66})}{(U_3)_{av}(\Delta t)_{av3j}} . \qquad (45)$$

From Fig. 7c, we have

$$x_1^{67} - x_3^{66} = x_1^{66} - \frac{x_1^{66} + 2 - x_3^{66}}{2} - x_3^{66} ,$$

$$x_1^{68} - T_F = x_3^{66} - 2 - T_F ,$$

$$(\Delta t)_{av3j} = \frac{(x_1^{67} - x_3^{66}) + (x_1^{68} - T_F)}{2} = \frac{x_1^{66} + x_3^{66} - 2T_F - 6}{4} \quad (46)$$

where T_F = temperature of the make-up feed.

Substituting equation (46) into equation (45), we obtain

$$A_{3j} = \frac{4F(1+r_3)(C_p)_{f3}(x_1^{66} + 2 - x_3^{66})}{(U_3)_{av}(x_1^{66} + x_3^{66} - 2T_F - 6)}$$

Again, multiplication of A_{3j} by $2C_3/F$ yields

$$(x_4)_{3j} = \frac{8C_3(1+r_3)(C_p)_{f3}(x_1^{66} + 2 - x_3^{66})}{(U_3)_{av}(x_1^{66} + x_3^{66} - 2T_F - 6)} . \quad (47)$$

Since the final stage of the third effect is under vacuum, pumping work is required for discharging the distillate and blowdown, the minimum pumping head required is,

$$\frac{\Delta P}{\rho} = \frac{P_{atm} - P_3}{\rho}$$

in which P_{atm} stands for the atmospheric pressure. The pumping cost is

$$(x_4)_{DC} = \frac{2C_4 \times (14.7 - P_3) \times 144}{62.5 \times 550 \times 3600 \times 0.85} \quad (48)$$

Since the plant is assumed to be located 50 feet above sea level, the theoretical pumping head required is

$$\frac{\Delta P_o}{\rho} + 50 = \frac{P_o - 14.7}{\rho} + 50 = \Delta H_o + 50 \qquad (49)$$

where the first term is the head difference which should be overcome in order to pump the make-up feed to the point corresponds to the maximum brine temperature. A correction factor of 1.18 should be attached to that to take account of the pumping efficiency. $(\frac{1}{0.85} = 1.18)$.
Therefore, the pumping cost is written as

$$(x_4)_{FP} = \frac{2C_4 \times 1.18(\Delta H_o + 50)}{550 \times 3600} \qquad (50)$$

The fixed charge cost for the structure for 50×10^6 gallons/day is

$$\text{unit structure cost} = \frac{2.3}{34} \times 10^6 = 0.0676 \times 10^6 \text{ (\$/stage)},$$

$$\text{total structure cost} = 0.0676 \times 68 \times 10^6 \text{ (\$)}$$

or

$$\text{capital charged cost} = 0.0676 \times 68 \times 10^6 \times 9.4 \times 10^{-6} \text{ (\$/hr)}$$

$$= 43.2 \text{ (\$/hr)}$$

where 9.4×10^{-6} is the capital charge constant based on the plant life of 20 years. Hence

$$(x_4)_{Str} = \frac{43.2}{\frac{62.4 \times 5 \times 10^7}{7.48 \times 24}} = \frac{(43.2)(7.48)(24)}{(62.4)(5)(10^7)} \text{ (\$/lb)} \qquad (51)$$

We are now able to write the accumulated cost as

$$x_4^{68} = x_4^{66} + (x_4)_{3j} + (x_4)_{DC} + (x_4)_{r3} .$$

where x_4^{66} is the accumulated cost for 66 stages, $(x_4)_{3j}$ is the cost of condenser tube area for the heat rejection section of the third effect, $(x_4)_{DC}$ is the cost required to discharge the distillate and blowdown, and $(x_4)_{r3}$ is

the cost of recycle in the third effect. In addition to this, we must consider the pumping cost of the feed, $(x_4)_{FP}$, and the cost of the structure, $(x_4)_{Str}$, that is,

$$(x_4)_T = x_4^{68} + (x_4)_{FP} + (x_4)_{Str} \tag{52}$$

The above cost is in dollars per pound. In units of dollars per 1000 gallons we can write

$$C_T = \frac{(x_4)_T \times 10^3 \times 62.4}{7.48}$$

The above mentioned cost items include only the in-plant operating and capital charge cost. Additional cost items should be included to calculate the total production cost. They are obtained from Ref. (3) and are listed in Table 1.

The design equations are presented in table form in Table 3.

3. RESULTS OF THE SIMULATION ACCORDING TO THE MICRO STAGE MODEL.

The simulation was carried out for two sets of variables on an IBM 1620 computer. The ranges of variables are listed in Table 4. For the first simulation study, the set of variables that was used is*

$$\Delta t_1 = 8.00^{\circ}F ,$$
$$\theta^{1n} = 2.00^{\circ}F ,$$
$$\theta^{2n} = 2.17^{\circ}F ,$$
$$\theta^{3n} = 2.38^{\circ}F .$$

For the second simulation study the set of variables is

---

*We assumed equal θ^n for each stage within an effect.

TABLE 1

DIRECT AND FIXED PRODUCTION COST AND GENERAL EXPENSES

Chemicals for pretreatment	$0.027
Supplies & Maintenance materials	$0.018
Labor	$0.038
General & Administrative Overhead	$0.011
Taxes & Insurance	$0.073
Interest on working capital	$0.005
Total per 10^3 gallons	$0.172

TABLE 2

NOMENCLATURE (THE MICROSTAGE MODEL)

C_1	unit steam cost	\$/lb
C_2	unit fixed charge cost for the brine heater	\$/ft^2 hr
C_3	unit fixed charge cost for the condenser tubes	\$/ft^2 hr
C_4	unit pumping cost	\$/H.P. hr
$(C_p)_{f1}$	heat capacity of the flashing brine, the first effect	BTU/lb ^oF
$(C_p)_{f2}$	heat capacity of the flashing brine, the second effect	BTU/lb ^oF
$(C_p)_{r1}$	heat capacity of recycle brine, the first effect	BTU/lb ^oF
F	amount of make-up feed	lb/hr
P_0	initial flashing pressure	lb/in^2
P_1	blowdown pressure of the first effect	lb/in^2
P_2	blowdown pressure of the second effect	lb/in^2
P_3	final blowdown pressure	lb/in^2
r_1	ratio of recycle brine in the first effect to the make-up feed	lb/lb
r_2	ratio of recycle brine in the second effect to the make-up feed	lb/lb
r_3	ratio of recycle brine in the third effect to the make-up feed	lb/lb
U_B	overall heat transfer coefficient of the brine heater	BTU/ft^{2}hr^{o}F
$(U_1)_{av.}$	average overall heat transfer coefficient of the condenser tubes, the first effect	BTU/ft^{2}hr^{o}F
$(U_2)_{av.}$	average overall heat transfer coefficient of the condenser tubes, the second effect	BTU/ft^{2}hr^{o}F
$(U_3)_{av.}$	average overall heat transfer coefficient of the condenser tubes, the third effect	BTU/ft^{2}hr^{o}F
ΔH_0	pumping head required for the make-up feed	ft

TABLE 2 (Cont'd)

Δt_1	temperature rise through the brine heater	^oF
Δt_{BPE}	boiling point elevation of the flashing brine	^oF
x_1	temperature of distillate	^oF
x_2	amount of distillate	lb/hr
x_3	temperature of recycle brine	^oF
x_4	unit production cost	$/lb
λ_s	latent heat of steam	BTU/lb
θ	temperature drop of distillate at each stage	^oF

TABLE 3

DESIGN EQUATIONS (THE MICROSTAGE MODEL)

Brine heater

(1) Steam cost

$$\frac{2C_1(1+r_1)(C_p)_{r1} \times \Delta t_1}{\lambda_s} \qquad (17)$$

$(C_p)_{r1}$, C_1, λ_s; given

Δt_1 : assumed

r_1 : calculated

(2) Fixed charge cost for the brine heater

$$\frac{2C_2(1+r_1)(C_p)_{r1}(\ln(24.4 + \Delta t_1) - \ln(24.4))}{U_B} \qquad (18)$$

C_2 : given

U_B : given

The first effect

heat recovery section

(1) Temperature of distillate

$$x_1^n = x_1^{n-1} - \theta^n \ , \ n = 1, 2, \ldots, 20 \qquad (8)$$

$$x_1^0 = T_f^o - \Delta t_{B.P.E.}$$

T_f^o : assumed

$\Delta t_{B.P.E.}$: given

θ^n : assumed

TABLE 3 (Cont'd)

(2) Amount of distillate

$$x_2^n = x_2^{n-1} + \frac{\left\{F(1+r_1) - x_2^{n-1}\right\}(C_p)_{f1}\,\theta^n}{x^n}$$

$$n = 1, 2, \ldots, 20 \qquad (9)$$

$x_2^0 = 0$: given

F : given

$(C_p)_{f1}$: given

$$\lambda^n = 1098.3 - 0.611x_1^n$$

(3) Temperature of recycle brine

$$x_3^n = x_3^{n-1} - \frac{\left\{F(1+r_1)(C_p)_{f1} + x_2^{n-1}(1-(C_p)_{f1}\right\}\theta^n}{F(1+r_1)(C_p)_{r1}} \qquad (14)$$

$$n = 1, 2, \ldots, 20$$

$$x_3^0 = (T_f)_{max} - \Delta t_1$$

(4) Fixed charge cost for condenser tubes

$$\frac{2C_3(1+r_1)(C_p)_{r1}\left\{\ln(x_1^{n-1}-\theta^n-x_3^n) - \ln(x_1^{n-1}-\theta^n-x_3^{n-1})\right\}}{(U_1)_{av.}}$$

$$n = 1, 2, \ldots, 20 \qquad (19)$$

$(U_1)_{av.}$: given

C_3 : given

TABLE 3 (Cont'd)

(2) Amount of distillate

$$x_2^n = x_2^{n-1} + \frac{\left\{F(5/6 + r_2) - x_2^{n-1}\right\}(C_p)_{f2}\,\theta^n}{1098.3 - 0.611\,x_1^n} \qquad (28)$$

$$n = 24, \ldots, 43$$

$x_2^{23} = 0$: given

$(C_p)_{f2}$: given

r_2 : calculated

(3) Temperature of feed and recycle brine

$$x_3^n = x_3^{n-1} - \frac{\left\{F(5/6+r_2)(C_p)_{f2} + x_2^{n-1}(1-(C_p)_{f2}) + F/6\right\}\theta^n}{F(0.965 + r_2 \times 0.9475)}$$

$$n = 24, \ldots, 43 \qquad (29)$$

$$x_3^{23} = x_3^{20} - \frac{(1+r_1)(C_p)_{f1}(x_1^{20}+2-x_3^{20})}{0.965 + r_2 \times 0.9475} \qquad (22)$$

(4) Fixed charge cost for condenser tubes

$$\frac{2C_3(0.965+r_2 \times 0.9475)(\ln(x_1^{n-1}-\theta^n-x_3^n)-\ln(x_1^{n-1}-\theta^n-x_3^{n-1}))}{(U_2)_{av.}}$$

$$n = 24, \ldots, 43 \qquad (30)$$

$(U_2)_{av.}$: given

TABLE 3 (Cont'd)

The first effect — heat rejection section

(1) Total amount of distillate

$$\frac{\left\{F(1+r_1) - x_2^{20}\right\}(C_p)_{f1}(x_1^{20} + 2 - x_3^{20})}{1098.3 - 0.3055(x_1^{20} + x_3^{20} + 2)} \qquad (23)$$

(2) Fixed charge cost for condenser tubes

$$\frac{12C_3(1+r_1)(C_p)_{f1}(x_1^{20} + 2 - x_3^{20})}{3(x_3^{20} - x_3^{23}) + 2(x_1^{20} - x_3^{20} - 8)\,(U_1)_{av.}} \qquad (26)$$

(3) Cost of recycle

$$\frac{2 \times C_4 \times r_1 \times 144\,(P_0 - P_1)}{62.5 \times 550 \times 3600 \times 0.85} \qquad (20)$$

where

P_0 : given

$$P_1 = \exp\left(14.07 - \frac{9 \times 3660}{5(x_3^{20} - 32) + 1989}\right)$$

The second effect — heat recovery section

(1) Temperature of distillate

$$x_1^n = x_1^{n-1} - \theta^n, \quad n = 24, \ldots, 43 \qquad (27)$$

θ^n : assumed

TABLE 3 (Cont'd)

The second effect — heat rejection section

(1) Total amount of distillate

$$\frac{\left\{F\left(\frac{5}{6} + r_2\right) - x_2^{43}\right\}(C_p)_{f2}(x_1^{43} + 2 - x_3^{43})}{1098.3 - 0.3055(x_1^{43} + 2 + x_3^{43})} \qquad (34)$$

(2) Fixed charge cost for condenser tubes

$$\frac{12C_3(1+r_2)(C_p)_{f2}(x_1^{43} + 2 - x_3^{43})}{\left\{3(x_3^{43} - x_3^{46}) + 2(x_1^{43} - x_3^{43}) - 8\right\}(U_2)_{av.}} \qquad (37)$$

(3) Cost of recycle

$$2 \times C_4 \times r_2 \times \frac{144}{62.5} \times \frac{(P_1 - P_2)}{550 \times 3600 \times 0.85} \qquad (31)$$

$$P_2 = \exp\left(14.07 - \frac{9 \times 3660}{5(x_3^{43} - 32) + 1989}\right)$$

The third effect — heat recovery section

(1) Temperature of distillate

$$x_1^n = x_1^{n-1} - \theta^n, \quad n = 47, \ldots, 66 \qquad (38)$$

θ^n : assumed

(2) Amount of distillate

$$x_2^n = x_2^{n-1} + \frac{\left\{F\left(\frac{2}{3} + r_3\right) - x_2^{n-1}\right\}(C_p)_{f3}\,\theta^n}{1098.3 - 0.611\,x_1^n} \qquad (39)$$

$n = 47, \ldots, 66$

$(C_p)_{f3}$: given

TABLE 3 (Cont'd)

r_3 : calculated

$x_2^{46} = 0$: given

(3) Temperature of feed and recycle brine

$$x_3^n = x_3^{n-1} - \frac{\left\{F(\frac{2}{3} + r_3)(C_p)_{f3} + x_2^{n-1}(1-(C_p)_{f3}) + \frac{F}{3}\right\}\theta^n}{F(0.965 + r_3 \times 0.93)}$$

$$n = 47, \ldots, 66 \qquad (40)$$

(4) Fixed charge cost for condenser tubes

$$x_3^{46} = x_3^{43} - \frac{(1+r_3)(C_p)_{f2}(x_1^{43} + 2 - x_3^{43})}{0.965 + r_3 \times 0.93} \qquad (33)$$

$$\frac{2C_3(0.965+r_3x0.93)(\ln(x_1^{n-1}-\theta^n-x_3^n)-\ln(x_1^{n-1}-\theta^n-x_3^{n-1}))}{(U_3)_{av.}}$$

$$n = 47, \ldots, 66 \qquad (41)$$

$(U_3)_{av.}$: given

The third effect

heat rejection section

(1) Total amount of distillate produced

$$\frac{\left\{F(\frac{2}{3} + r_3) - x_2^{66}\right\}(C_p)_{f3}(x_1^{66} + 2 - x_3^{66})}{1098.3 - 0.3055(x_1^{66} + 2 - x_3^{66})} \qquad (44)$$

(2) Fixed charge cost for condenser tubes

$$\frac{8C_3(1+r_3)(C_p)_{f3}(x_1^{66} + 2 - x_3^{66})}{(x_1^{66} + x_3^{66} - 172)(U_3)_{av.}} \qquad (47)$$

TABLE 3 (Cont'd)

(3) Cost of recycle

$$2 \times C_4 \times r_3 \times \frac{144}{62.5} \times \frac{P_2 - P_3}{550 \times 3600 \times 0.85} \quad (44)$$

$$P_3 = \exp\left(14.07 - \frac{9 \times 3660}{5(x_3^{66} - 32) + 1989}\right)$$

Others

(1) Pumping cost for the make-up feed

$$\frac{2C_4\left(\frac{H_0}{0.85} + \frac{50}{0.85}\right)}{550 \times 3600} \quad (50)$$

H_0 : given (steam table)

(2) Pumping cost for the distillate and blowdown

$$2 \times C_4 \times \frac{144}{62.5} \times \frac{14.7 - P_3}{550 \times 3600 \times 0.85} \quad (48)$$

(3) Structure cost for the whole system

Total structure cost = c_5 x No. of stages

$$\text{fixed charge cost} = \frac{\text{total structure cost} \times 9.4 \times 10^{-6}}{\frac{62.4 \times 5 \times 10^7}{7.48 \times 24}} \quad (51)$$

C_5 : given

TABLE 3 (Cont'd)

Summary

Unit production cost includes:

(1) steam cost

(2) fixed charge cost for the brine heater

(3) fixed charge cost for the condenser tubes in each effect

(4) cost of recycle for each effect (includes power and depreciation of pumps)

(5) pumping cost for the make-up feed (includes power and depreciation)

(6) pumping cost for the distillate and blowdown (includes power and depreciation)

(7) structure cost for the whole system

TABLE 4

UNIT COSTS USED IN THIS STUDY

1. Steam cost

   Steam cost = \$0.25/1000 lb

   or c_1 = $\$2.5 \times 10^{-4}$/lb

2. Fixed charge cost for the brine heater*

   Unit price of the brine heater = $\$4/ft^2$

   $c_2 = 4 \times 9.4 \times 10^{-6} = \$3.76 \times 10^{-5}/ft^2$ hr

3. Fixed charge cost for the condenser tubes

   Unit price of the condenser tubes = $\$2.55/ft^2$

   $c_3 = 2.55 \times 9.4 \times 10^{-6} = \$2.397 \times 10^{-5}/ft^2$ hr

4. Pumping cost

   Unit price of pumps = \$85/HP

   Pump depreciation cost = $85 \times 9.4 \times 10^{-6} = \$8 \times 10^{-4}$/HP hr

   Power cost = 0.69¢/KWH = $\$5.2 \times 10^{-3}$/HP hr

   c_4 = pump depreciation + power cost = $\$6.0 \times 10^{-3}$/HP hr

---

*9.4×10^{-6} is the proportionality constant of depreciation based on the plant life of 20 years with 90% stream days and an annual interest of 4%.

TABLE 5

RANGE OF VARIABLES (THE MACROSTAGE MODEL)

	Variable name	Unit	Range
1.	Temperature of flashing brine	^{o}F	$87 < T_F < 274.4$
2.	Temperature of distillate	^{o}F	$85 < x_1 < 272.4$
3.	Temperature of recycle brine	^{o}F	$85 < x_3 < 272.4$
4.	Temperature difference between the flashing and recycle brine (before flashing)	^{o}F	$2 < \Delta t_1 < 15$
5.	Concentration of the flashing brine	wt.%	$3.5 < C_f \leq 7.0$
6.	Temperature drop of the distillate	^{o}F	$\theta_1^n < x_1^n - x_3^n$
7.	Temperature drop of the distillate in each stage in the second effect	^{o}F	$\theta_2^n < x_1^n - x_3^n$
8.	Temperature drop of the distillate in each stage in the third effect	^{o}F	$\theta_1^n < x_1^n - x_3^n$

$$\Delta t_1 = 9.00^{\circ}F ,$$
$$\theta^{1n} = 1.85^{\circ}F ,$$
$$\theta^{2n} = 2.17^{\circ}F ,$$
$$\theta^{3n} = 2.48^{\circ}F .$$

The computer flow diagram is given in Fig. 9, and the computer program symbols and the computer program are listed in Table 6. The results for both cases are tabulated in Table 7. Since it takes time to repeat the computation, the macro stage model was used for the subsequent simulation studies.

It should be pointed out that the determination of the recycle ratio for each effect is achieved by an iteration procedure. For a fixed range of flashing temperature and for a fixed distillate production, the recycle ratio becomes a dependent variable so that it can be evaluated by an iterative procedure for the conditions chosen. In this study, a value of the recycle ratio was assumed and the total distillate production for that effect was calculated until a distillate production of $\frac{F}{6}$ was obtained.

4. FORMULATION OF THE DESIGN EQUATIONS ACCORDING TO THE MACRO STAGE MODEL.

In this section, we will consider the design equations for the macro-stage system. The only difference between the macro-stage and micro-stage system is that in the former we consider the performance of the heat recovery section as a whole unit, while in the latter we go into more detail by considering the performance at each stage within the heat recovery section. The basis of the formulation is a 50 million gallon per day plant. It is assumed that the salt water fed to the system contains 3.5 weight per cent salt and that the concentrated brine leaving the system (blowdown) contains 7 weight per cent salt. This information is presented together with other numerical

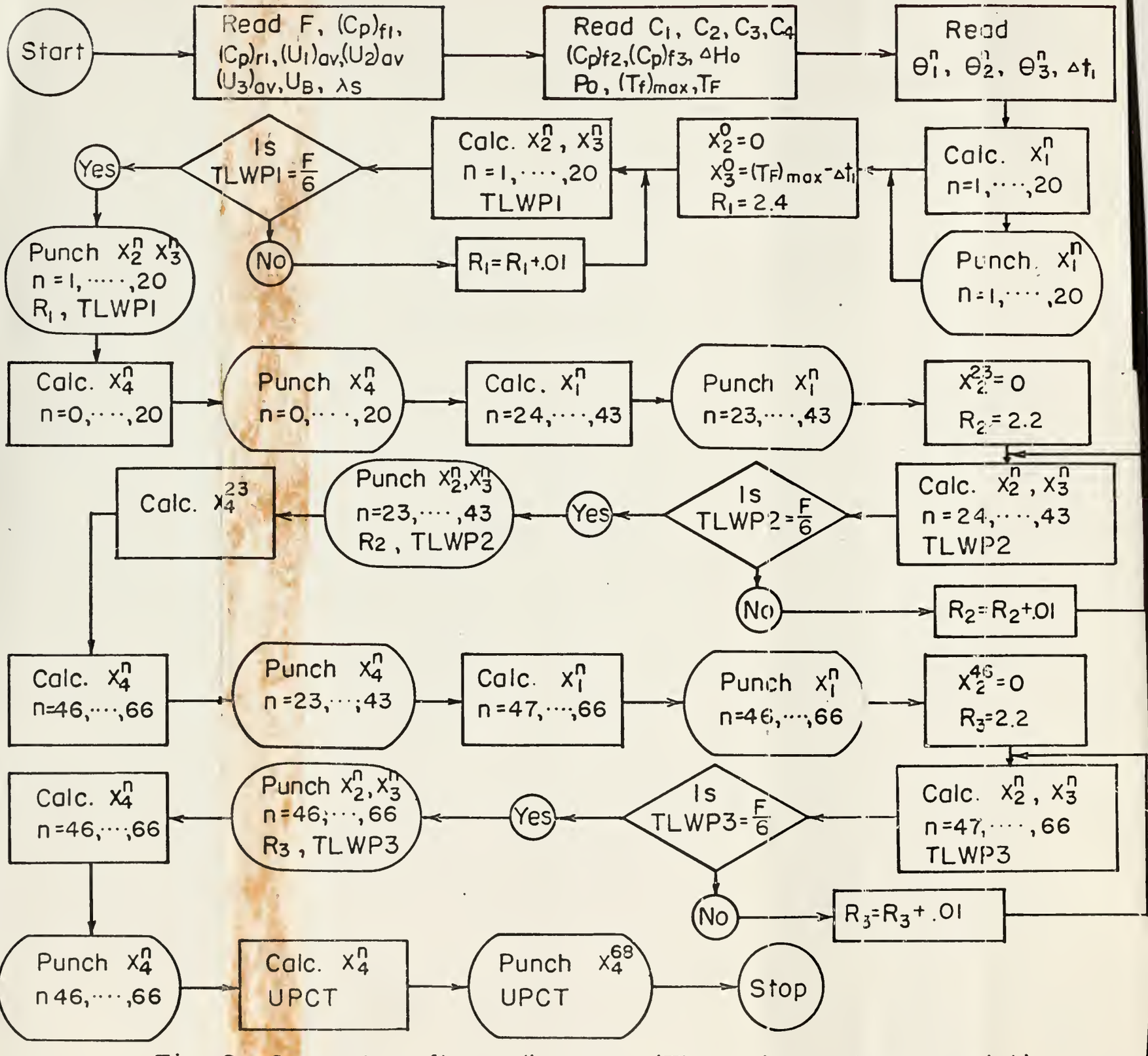


Fig. 9 Computer flow diagram (The micro stage model).

TABLE 6

A. EXPLANATION OF PROGRAMMING SYMBOLS

(THE MICROSTAGE MODEL)

Symbol	Explanation
BHACT	fixed charge cost for the brine heater
C1	unit steam cost
C2	unit fixed charge cost for the brine heater
C3	unit fixed charge cost for the condenser tubes
C4	unit pumping cost
CPF1	average heat capacity of the flashing brine, the first effect
CPF2	average heat capacity of the flashing brine, the second effect
CPF3	average heat capacity of the flashing brine, the third effect
CPR1	heat capacity of recycle brine, the first effect
DCCT	pumping cost for the distillate and blowdown
DELHO	pumping head for the make-up feed
DELT1	temperature rise through the brine heater
FD	amount of make-up feed
FT	temperature of make-up feed
FBCT1	cost of recycle, the first effect
FBCT2	cost of recycle, the second effect
FBCT3	cost of recycle, the third effect
FPCT	pumping cost for the make-up feed
HFT	maximum brine temperature
HJCT1	fixed charge cost for the condenser tubes, heat rejection section, the second effect

TABLE 6 (Cont'd)

HJCT2	fixed charge cost for the condenser tubes, heat rejection section, the second effect
HJCT3	fixed charge cost for the condenser tubes, heat rejection section, the third effect
PO	initial flashing pressure
P1	blowdown pressure, the first effect
P2	blowdown pressure, the second effect
P3	blowdown pressure, the third effect
R1	ratio of recycle brine in the first effect to the make-up feed
R2	ratio of recycle brine in the second effect to the make-up feed
R3	ratio of recycle brine in the third effect to the make-up feed
STMCT	steam cost
STRCT	structure cost
THIN	temperature drop of the distillate in each stage, heat recovery section, the first effect
TH2N	temperature drop of the distillate in each stage, heat recovery section, the second effect
TH3N	temperature drop of the distillate in each stage, heat recovery section, the third effect
TLWP1	total distillate production in the first effect
TLWP2	total distillate production in the second effect
TLWP3	total distillate production in the third effect
UB	overall heat transfer coefficient of the brine heater
UIAV	average overall heat transfer coefficient of the condenser tubes, the first effect

TABLE 6 (Cont'd)

U2AV	average overall heat transfer coefficient of the condenser tubes, the second effect
U3AV	average overall heat transfer coefficient of the condenser tubes, the third effect
UPCT	unit production cost
X1	temperature of distillate
X2	amount of distillate
X3	temperature of recycle brine
X4	unit production cost (lb basis)
X4BH	production cost due to the brine heater

B. SIMULATION OF THE MULTIFLASH EVAPORATION PROCESS (THE MICROSTAGE MODEL)

```
      DIMENSION X1(70),X2(70),X3(70),X4(70)
  101 FORMAT(6X,6E10.4)
   16 FORMAT(2X,7F10.3)
   26 FORMAT(2X,7E10.4)
   27 FORMAT(F10.3,E10.4)
   60 FORMAT(2E10.4)
      READ 101,FD,CPF1,CPR1,U1AV,U2AV,U3AV
      READ 101,C1,C2,C3,C4,CPF2,CPF3
      READ 101,UB,RMS,DELH0,P0,HFT,FT
      READ 101,TH1N,TH2N,TH3N,DELT1
C     CALC,X1(I)
      X1(1)=248.0
      DO 11 I=2,21
   11 X1(I)=X1(I-1)-TH1N
      PUNCH 16,(X1(I),I=1,21)
C     CAL,X2(I),X3(I)
      X2(1)=0.0
      X3(1)=HFT -DELT1
      R1=2.4
   22 DO 21 I=2,21
      X2(I)=X2(I-1)+(FD*(1.+R1)-X2(I-1))*CPF1*TH1N/(1098.3-.611*X1(I))
   21 X3(I)=X3(I-1)-(FD*(1.+R1)*CPF1+X2(I-1)*(1.-CPF1))*TH1N/(FD*(1.+R1)
     1*CPR1)
      TLWP1=X2(21)+ FD*(1.+R1)*CPF1*(X1(21)+2.-X3(21))/(1098.3-.3055*(X1
     1(21)+X3(21)+2.))
      IF (TLWP1-FD/6.) 31,32,32
   31 R1=R1+.01
      GO TO 22
   32 PUNCH 26,(X2(I),I=1,21)
      PUNCH 16,(X3(I),I=1,21)
      PUNCH 27,R1, TLWP1
C     CALC,X4(I)
      STMCT=2.*C1*(1.+R1)*DELT1*CPR1/RMS
      BHACT=(LOG(24.4+DELT1)-LOG(24.4))*(1.+R1)*2.*C2*CPR1/UB
      X4BH=STMCT+BHACT
      X4(1)=X4BH



      DO 41 I=2,21
   41 X4(I)=X4(I-1)+2.*C3*(1.+R1)*CPR1*(LOG(X1(I-1)-TH1N-X3(I))-LOG(X1(I
     1-1)-TH1N-X3(I-1)))/U1AV
      PUNCH 46,(X4(I),I=1,21)
```

(CONTINUED)

```
C       CALC(X1(I) I=25,44
        X1(24)=X3(21)-2.
        DO 12 I=25,44
   12   X1(I)=X1(I-1)-TH2N
        PUNCH 16,(X1(I),I=24,44)
C       CALC,X2(I) ,X3(I)
        X2(24)=0.0
        R2=2.2
   24   X3(24)=X3(21)-(1.+R1)*CPF1*( X1(21)+2.-X3(21))/(.965+R2*.9475)
        DO 23 I=25,44
         X2(I)= X2(I-1)+(FD*(5./6.+R2)- X2(I-1))*CPF2*TH2N/(1098.3-.611*X1
       1(I))
   23   X3(I)=X3(I-1)-(FD*(5./6.+R2)*CPF2+X2(I-1)*(1.-CPF2)+ FD/6.)*TH2N/
       1(F D*(.965+R2*.9475))
        TLWP2=X2(44)+FD*(1.+R2)*CPF2*(X1(44)+2.-X3(44))/(1098.3-.3055*(X1
       1(44)+X3(44)+2.))
        IF(TLWP2-FD/6.) 33,34,34
   33   R2=R2+.01
        GO TO 24
   34   PUNCH 26,(X2(I), I=24,44)
        PUNCH 16,(X3(I),I=24,44)
        PUNCH 27,R2,TLWP2
C       CAL.X4(I)
        HJCT1=12.*C3*(1.+R1)*CPF1*(X1(21)+2.-X3(21))/(3.*(X3(21)-X3(24))+
       12.*(X1(21)-X3(21))-8.)/U1AV
        P1=EXP(14.07-9.*3660./(5.*(X3(21)-32.)+1989.))
        FBCT1=2.*C4*R1*144.*(P0-P1)/62.5/550./3600./.85
        X4(24)=X4(21)+HJCT1+FBCT1
        DO 42 I=25,44
   42   X4(I)=X4(I-1)+2.*C3*(.965+R2*.9475)*(LOG(X1(I-1)-TH2N-X3(I))-LOG
       1(X1(I-1)-TH2N-X3(I-1)))/U2AV
        PUNCH 26,(X4(I),I=24,44)
C       CALC.X1(I) I=48,67
        X1(47)=X3(44)-2.
        DO 13 I=48,67
   13   X1(I)=X1(I-1)-TH3N
        PUNCH 16,(X1(I),I=47,67)
C       CAL.X2(I),X3(I) I=47,67
        X2(47)=0.0
        R3=2.2
   51   X3(47)=X3(44)-(1.+R2)*CPF2*(X1(44)+2.-X3(44))/(.965+R3*.930)
        DO 52 I=48,67
        X2(I)=X2(I-1)+(FD*(2./3.+R3)-X2(I-1))*CPF3*TH3N/(1098.3-.611*X1(I)
       1)
   52   X3(I)=X3(I-1)-(FD*(2./3.+R3)*CPF3+X2(I-1)*(1.-CPF3)+FD/3.)*TH3N/
       1(FD*(.965+R3*.930))
        TLWP3=X2(67)+FD*(1.+R3)*CPF3*(X1(67)+2.-X3(67))/(1098.3-.3055*(X1
       1(67)+X3(67)+2.))
        IF (TLWP3-FD/6.) 53,54,54
   53   R3=R3+.01
        GO TO 51
```

(CONTINUED)

```
   54 PUNCH 26,(X2(I),I=47,67)
      PUNCH 16,(X3(I),I=47,67)
      PUNCH 27,R3 ,TLWP3
C     CALC.X4(I) I=47,67
      HJCT2=12.*C3*(1.+R2)*CPF2*(X1(44)+2.-X3(44))/(3.*(X3(44)-X3(47))+
     12.*(X1(44)-X3(44))-8.)/U2AV
      P2=EXP(14.07-9.*3660./(5.*(X3(44)-32.)+1989.))
      FBCT2=2.*C4*R2*144.*(P1-P2)/62.5/550./3600./.85
      X4(47)=X4(44)+HJCT2+FBCT2
      DO 43 I=48,67
   43 X4(I)=X4(I-1)+2.*C3*(.965+R2*.93)*(LOG(X1(I-1)-TH3N-X3(I))-LOG(X1
     1(I-1)-TH3N-X3(I-1)))/U3AV
      PUNCH 26,(X4(I),I=47,67)
      HJCT3=8.*C3*(1.+R3)*CPF3*(X1(67)+2.-X3(67))/(X1(67)+X3(67)-2.*FT-
     16.)/U3AV
      P3=EXP(14.07-9.*3660./(5.*(X3(67)-32.)+1989.))
      FBCT3=2.*C4*R3*144.*(P2-P3)/62.5/550./3600./.85
      DCCT=2.*C4*144.*(14.7-P3)/62.5/550./3600./.85
      X4(69)=X4(67)+HJCT3+FBCT3+DCCT
C     CALC.UPCT
      FPCT =2.*C4*1.18*(DELH0+50.)/550./3600.
      STRCT=43.2*7.48*24./(62.4*5.E7)
      UPCT=(X4(69)+FPCT+STRCT)*1.E3*62.4/7.48
      PUNCH 60,X4(69),UPCT
      END
      DATA
       .3476E 08 .9590E 00 .9590E 00 .5150E 03 .5100E 03 .5050E 03
       .2500E-03 .3760E-04 .2397E-04 .6000E-02 .9485E 00 .9310E 00
       .5371E 03 .9289E 03 .3480E 02 .2982E 02 .2500E 03 .8500E 02
       .2000E 01 .2170E 01 .2380E 01 .8000E 01
       .1850E 01 .2170E 01 .2480E 01 .9000E 01
```

TABLE 7

RESULTS OF SIMULATION (THE MICROSTAGE MODEL)

Total number of effects	3
Total number of stages	68
Total production	17,380 Mlb/hr = 50. MMGPD
Maximum brine temperature	250.0 ^{o}F
Sea water temperature	85.0 ^{o}F
Sea water concentration	3.50 wt. %
Blow down brine concentration	7.00 wt. %
Sea water make-up	34,760 Mlb/hr

Case I: $\Delta t_1 = 8.0\ ^{o}F$, $\theta_1^n = 2.0\ ^{o}F$ $\theta_2^n = 2.17\ ^{o}F$ $\theta_3^n = 2.38\ ^{o}F$

Effect No.	No. of Stages	Production Mlb/hr	Recycle Brine, Mlb/hr	Blowdown Mlb/hr	Blowdown Temp. ^{o}F	Recycle Brine Conc. wt. %
1	23	5795	88986	28967	201.967	4.20
2	23	5799	92114	23173	150.638	5.25
3	22	5796	94896	17380	95.214	7.00

TABLE 7 (Cont'd)

Effect No.	Stage No.	Flashing Brine Temp. ^{o}F	Distillate Temp. ^{o}F	Recycle-make-up Brine Temp. ^{o}F	Distillate Mlb/hr	Accumulated Unit Production Cost $/lb x 10^5
	Brine Heater	---	---	242 250	---	1.483
1	1	248.000	246.000	240.000	250.3	1.496
	2	246.000	244.000	237.999	499.9	1.509
	3	244.000	242.000	235.999	748.6	1.522
	4	242.000	240.000	233.998	996.5	1.535
	5	240.000	238.000	231.998	1243.0	1.548
	6	238.000	236.000	229.997	1489.0	1.561
	7	236.000	234.000	227.996	1735.0	1.573
	8	234.000	232.000	225.995	1979.0	1.586
	9	232.000	230.000	223.993	2223.0	1.599
	10	230.000	228.000	221.992	2466.0	1.612
	11	228.000	226.000	219.990	2709.0	1.625
	12	226.000	224.000	217.988	2950.0	1.638
	13	224.000	222.000	215.986	3191.0	1.651
	14	222.000	220.000	213.984	3431.0	1.664
	15	220.000	218.000	211.982	3670.0	1.676
	16	218.000	216.000	209.070	3908.0	1.689
	17	216.000	214.000	207.976	4146.0	1.702
	18	214.000	212.000	205.974	4382.0	1.715
	19	212.000	210.000	203.971	4618.0	1.728
	20	210.000	208.000	201.967	4854.0	1.741

TABLE 7 (Cont'd)

Heat rejection section

21	↓	↓	↓	↓	↓
22	↓	↓	↓	↓	↓
23	201.967	199.967	194.078	5795.0	1.872

TABLE 7 (Cont'd)

Effect No.	Stage No.	Flashing Brine Temp. ^{o}F	Distillate Temp. ^{o}F	Recycle-make-up Brine Temp. ^{o}F	Distillate Mlb/hr	Accumulated Unit Production Cost $/lb x 10^5
2	24	199.797	197.797	191.911	254.9	1.887
	25	197.627	195.627	189.745	509.0	1.902
	26	195.457	193.457	187.577	762.2	1.917
	27	193.287	191.287	185.410	1014.0	1.932
	28	191.117	189.117	183.242	1266.0	1.947
	29	188.947	186.947	181.074	1516.0	1.962
	30	186.777	184.777	178.906	1766.0	1.977
	31	184.607	182.607	176.738	2015.0	1.992
	32	182.437	180.437	174.569	2263.0	2.007
	33	180.267	178.267	172.401	2510.0	2.022
	34	178.097	176.097	170.232	2756.0	2.037
	35	175.927	173.927	168.062	3002.0	2.052
	36	173.757	171.757	165.893	3246.0	2.067
	37	171.587	169.587	163.723	3490.0	2.082
	38	169.417	167.417	161.553	3733.0	2.098
	39	167.247	165.247	159.383	3975.0	2.113
	40	165.077	163.077	157.213	4217.0	2.128
	41	162.907	160.907	155.042	4457.0	2.143
	42	160.737	158.737	152.871	4697.0	2.158
	43	158.567	156.567	150.700	4936.0	2.173
Heat rejection section						
	44	↓	↓	↓	↓	↓
	45					
	46	150.700	198.700	142.927	5799.0	2.265

TABLE 7 (Cont'd)

Effect No.	Stage No.	Flashing Brine Temp. ^{o}F	Distillate Temp. ^{o}F	Recycle-make-up Brine Temp. ^{o}F	Distillate Mlb/hr	Accumulated Unit Production Cost $/lb x 10^5
3	47	146.320	146.320	140.552	259.3	2.283
	48	145.940	143.940	138.178	517.6	2.300
	49	143.560	141.560	135.803	775.0	2.318
	50	141.180	139.180	133.427	1031.0	2.336
	51	138.800	136.800	131.051	1287.0	2.353
	52	136.420	134.420	128.675	1541.0	2.371
	53	134.040	132.040	126.299	1795.0	2.389
	54	131.660	129.660	123.922	2048.0	2.407
	55	129.280	127.280	121.545	2300.0	2.424
	56	126.900	124.900	119.168	2551.0	2.442
	57	124.520	122.520	116.790	2801.0	2.460
	58	122.140	120.140	114.412	3050.0	2.478
	59	119.760	117.760	112.033	3298.0	2.496
	60	117.380	115.380	109.654	3546.0	2.514
	61	115.000	113.000	107.275	3792.0	2.532
	62	112.620	110.620	104.896	4038.0	2.549
	63	110.240	108.240	102.516	4283.0	2.567
	64	107.860	105.860	100.136	4527.0	2.585
	65	105.480	103.480	97.755	4770.0	2.603
	66	103.100	101.100	95.374	5012.0	2.621
Heat rejection section						
	67	↓	↓	↓	↓	↓
	68	95.374	93.374	85.000	5796.0	2.707

unit production cost 0.2516 $/$10^3$ gallon

TABLE 7 (Cont'd)

Case II: $\Delta t_1 = 9\ ^{o}F\quad \theta_1^n = 1.85\ ^{o}F\quad \theta_2^n = 2.17\ ^{o}F\quad \theta_3^n = 2.48\ ^{o}F$

Effect No.	No. of Stages	Production Mlb/hr	Recycle Brine, Mlb/hr	Blowdown Mlb/hr	Blowdown Temp. ^{o}F	Recycle brine Conc. wt. %
1	23	5808	93504	28967	203,972	4.20
2	23	5800	86205	23173	150,962	5.25
3	22	5799	84467	17380	81,588	7.00

Effect No.	Stage No.	Flashing Brine Temp. ^{o}F	Distillate Temp. ^{o}F	Recycle-make-up Brine Temp. ^{o}F	Distillate Mlb/hr	Accumulated Unit Production Cost $/lb x 10^5
	Brine	---	---	241	---	1.739
	Heater	---	---	250	---	
1	1	248.150	246.150	239.150	241.3	1.749
	2	246.300	244.300	237.299	481.9	1.759
	3	244.450	242.450	235.449	721.8	1.769
	4	242.600	240.600	233.599	961.0	1.779
	5	240.750	238.750	231.748	1199.0	1.790
	6	238.900	236.900	229.897	1437.0	1.800
	7	237.050	235.050	228.046	1674.0	1.810
	8	235.200	233.250	226.195	1910.0	1.820
	9	233.350	231.350	224.344	2145.0	1.830
	10	231.500	229.500	222.493	2380.0	1.840
	11	229.650	227.650	220.641	2614.0	1.851
	12	227.800	225.800	218.790	2848.0	1.861

TABLE 7 (Cont'd)

Effect No.	Stage No.	Flashing Brine Temp. ^{o}F	Distillate Temp. ^{o}F	Recycle-make-up Brine Temp. ^{o}F	Distillate Mlb/hr	Accumulated Unit Production Cost $\$/lb \times 10^{5}$
	13	225.950	223.950	216.938	3081.0	1.871
	14	224.100	222.100	215.086	3313.0	1.881
	15	222.250	220.250	213.234	3544.0	1.891
	16	220.400	218.400	211.382	3774.0	1.901
	17	218.550	216.550	209.530	4004.0	1.911
	18	216.700	214.700	207.677	4234.0	1.922
	19	214.850	212.850	205.825	4462.0	1.932
	20	213.000	211.000	203.972	4690.0	1.942
	Heat rejection section					
	21	↓	↓	↓	↓	↓
	22					
	23	203.972	201.972	194.446	5798.0	2.072
2	24	201.802	199.802	192.279	247.2	2.083
	25	199.632	197.732	190.113	493.5	2.093
	26	197.462	195.462	187.946	739.1	2.104
	27	195.292	193.292	185.778	983.7	2.115
	28	193.122	191.122	183.611	1227.0	2.126
	29	190.952	188.952	181.443	1470.0	2.136
	30	188.782	186.782	179.275	1712.0	2.147
	31	186.612	184.612	177.107	1954.0	2.158
	32	184.442	132.442	174.939	2194.0	2.169
	33	182.272	180.272	172.770	2434.0	2.180

Effect No.	Stage No.	Flashing Brine Temp. °F	Distillate Temp. °F	Recycle-make-up Brine Temp. °F	Distillate Mlb/hr	Accumulated Unit Production Cost $/lb x 10^5
	34	180.102	178.102	170.601	2673.0	2.191
	35	177.932	175.932	168.432	2911.0	2.201
	36	175.762	173.762	166.263	3148.0	2.212
	37	173.592	161.592	164.093	3384.0	2.223
	38	171.422	169.422	161.923	3620.0	2.234
	39	169.252	167.252	159.753	3855.0	2.245
	40	167.082	165.082	157.583	4089.0	2.255
	41	164.912	162.912	155.413	4322.0	2.266
	42	162.742	160.742	153.242	4554.0	2.277
	43	160.572	158.572	151.071	4786.0	2.288
	Heat rejection section					
	44	↓	↓	↓	↓	↓
	45					
	46	151.071	149.071	141.430	5796.0	2.374
3	47	148.591	146.591	138.956	253.5	2.386
	48	146.111	144.111	136.482	506.1	2.398
	49	143.631	141.631	134.008	757.7	2.411
	50	141.151	139.151	131.533	1008.0	2.423
	51	138.671	136.671	129.058	1258.0	2.435
	52	136.191	134.191	126.582	1506.0	2.448
	53	133.711	131.711	124.106	1754.0	2.460
	54	131.231	129.231	121.630	2001.0	2.472
	55	128.751	126.751	119.153	2247.0	2.485

Effect No.	Stage No.	Flashing Brine Temp. ^{o}F	Distillate Temp. ^{o}F	Recycle-make-up Brine Temp. ^{o}F	Distillate Mlb/hr	Accumulated Unit Production Cost $/lb x 10^5
	56	126.271	124.271	116.676	2492.0	2.497
	57	123.791	121.791	114.199	2736.0	2.509
	58	121.311	119.311	111.721	2980.0	2.522
	59	118.831	116.831	109.243	3222.0	2.534
	60	116.351	114.351	106.765	3463.0	2.547
	61	113.871	111.871	104.286	3704.0	2.559
	62	111.391	109.391	101.807	3944.0	2.572
	63	108.911	106.911	99.327	4182.0	2.584
	64	106.431	104.431	96.847	4420.0	2.596
	65	103.951	101.951	94.367	4657.0	2.609
	66	101.471	99.471	91.887	4894.0	2.621
Heat rejection section						
	67	↓	↓	↓	↓	↓
	68	91.887	89.887	85.00	5803.0	2.735

Unit Production cost: 0.2539 $/$10^3$ gallon

data in Table 7.

(A) Design Equations for the First Effect. In this section only the design equations for the brine heater (bht) and the heat recovery section are given. The design equations for the heat rejection section are included in part (B). An energy balance for the first effect (refer to Fig. 10) gives

$$F(1+r_1)(C_{p1})_{av}\, x_0 = \frac{F}{6}(H_{v1})_{av} + F(\frac{5}{6} + r_1)(C_p)_{f1}\, x_1 \qquad (53)$$

where F = amount of make-up feed,

x = temperature of flashing brine (^oF)

$(H_{v1})_{av}$ = average enthalpy of water vapor in the first effect relative to liquid at 0^oF

H_v = $1065 + 0.392x$ (BTU/lb) (an empirical formula obtained by curve fitting the steam table).

$$(H_{v1})_{av} = \frac{1065 + 0.392x_0 + 1065 + 0.392x_1}{2}$$

$$= 1065 + 0.196(x_1 + x_0)$$

r_1 = ratio of the recycle brine in the first effect to the make-up feed

$$(C_{p1})_{av} = \frac{(C_p)_F + r_1(C_p)_{f1}}{1+r_1}$$

$(C_p)_F$ = heat capacity of the make-up feed,

$(C_p)_{f1}$ = heat capacity of the flashing brine at the exit of the first effect.

Simplifying and rewriting equation (53), we obtain

$$\{(C_p)_F + r_1(C_p)_{f1}\}x_0 = \frac{1}{6}\{1065 + 0.196(x_0 + x_1)\} + (\frac{5}{6} + r_1)(C_p)_{f1}x_1 .$$

Solving for r_1, we have

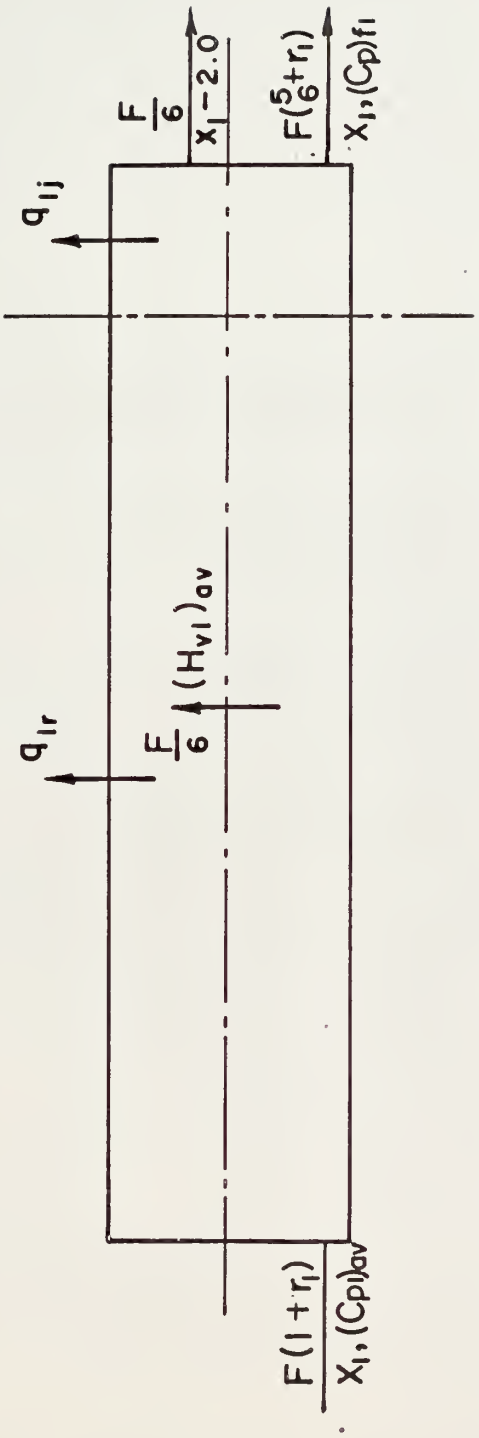


Fig. 10. Schematic flow diagram for the first effect.

$$r_1 = \frac{1065 + 0.196(x_0 + x_1) + 5(C_p)_{f1}x_1 - 6(C_p)_F x_0}{6(C_p)_{f1}(x_0 - x_1)} \quad (54)$$

For the steam that is used in the brine heater, the steam cost in dollars per pound of distillate product, $(x_4)_s$, is

$$(x_4)_s = \frac{2C_1(1+r_1)(C_p)_{av}\Delta t_1}{\lambda_s}$$

$$(x_4)_s = \frac{2C_1\{(C_p)_F + r_1(C_p)_{f1}\}\Delta t_1}{\lambda_s} \quad (55)$$

(See equation (17) in the micro-stage model.)

The fixed charge cost for the brine heater, $(x_4)_B$, is (see equation (18) in the micro-stage model)

$$(x_4)_B = \frac{2C_2(1+r_1)(C_{p1})_{av}}{U_B}\{\ln(24.4 + \Delta t_1) - \ln(24.4)\}$$

$$(x_4)_B = \frac{2C_2\{(C_p)_F + r_1(C_p)_{f1}\}}{U_B}\{\ln(24.4 + \Delta t_1) - \ln(24.4)\} \quad (56)$$

The rate of heat transfer for the condenser tubes of the heat recovery section of the first effect is

$$q_{1r} = F(1+r_1)(C_{p1})_{av}(x_0 - x_1 - \Delta t_1)$$

The heat transfer area, A_{1r}, is given by

$$A_{1r} = \frac{q_{1r}}{(U_1)_{av}(\Delta t_{1r})_{av}}$$

where

$$(\Delta t_{1r})_{av} = \frac{(\Delta t_1 - 2) + (\Delta t_1 - 2 - \frac{x_0 - x_1 - \Delta t_1}{20})}{2}$$

$$= \frac{41\ \Delta t_1 - x_0 + x_1 - 80}{40}$$

Hence, the fixed charge cost, $(x_4)_{c1}$, is

$$(x_4)_{c1} = \frac{C_3 F\{(C_p)_F + r_1(C_p)_{f1}\}(x_0 - x_1 - \Delta t_1)}{\frac{F}{2}(U_1)_{av}\left(\frac{41\Delta t_1 - x_0 + x_1 - 80}{40}\right)}$$

$$(x_4)_{c1} = \frac{80 C_3\{(C_p)_F + r_1(C_p)_{f1}\}(x_0 - x_1 - \Delta t_1)}{(U_1)_{av}(41\Delta t_1 - x_0 + x_1 - 80)} . \qquad (57)$$

The recycle cost for the first effect, $(x_4)_{r1}$ is (see equation (20) for the micro-stage model)

$$(x_4)_{r1} = \frac{2C_4 r_1 \times 144(P_0 - P_1)}{62.5 \times 550 \times 3600 \times 0.85} . \qquad (58)$$

where

$$P_1 = \exp\left\{14.07 - \frac{9 \times 3660}{5(x_1 - 32) + 1989}\right\}$$

(B) Design Equations for the Second Effect. Making an energy balance for the second effect (refer to Fig. 11), we have

$$F\left(\frac{5}{6} + r_2\right)(C_{p2})_{av} x_1 = \frac{F}{6}(H_{v2})_{av} + F\left(\frac{2}{3} + r_2\right)(C_p)_{f2} x_2 \qquad (59)$$

Since

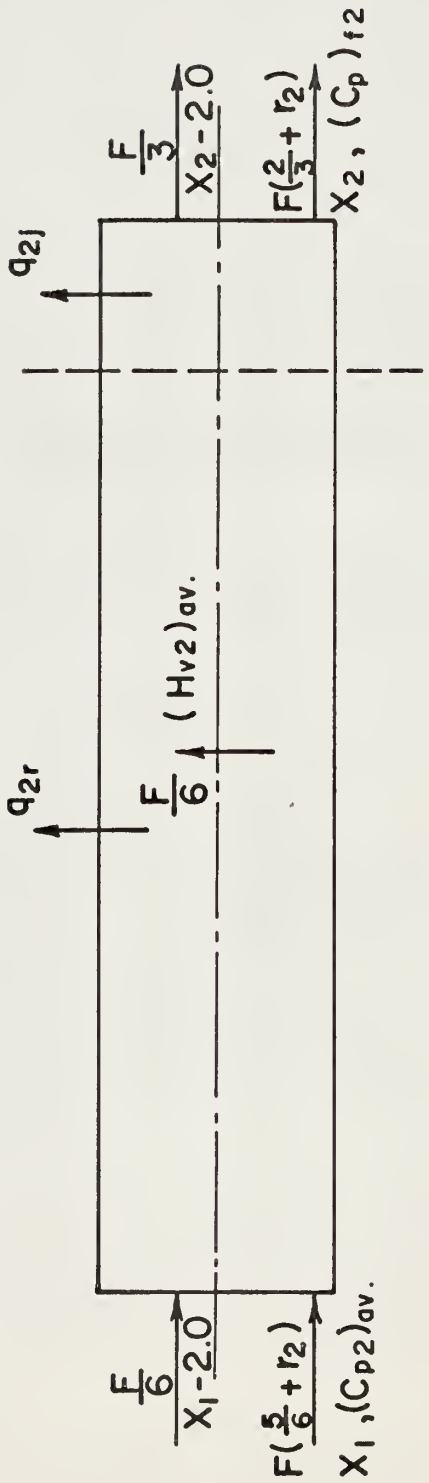


Fig. 11. Schemetic flow diagram for the second effect.

$$(C_{p2})_{av} = \frac{\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2}}{\frac{5}{6} + r_2} ,$$

$$(H_{v2})_{av} = 1065 + 0.196(x_1 + x_2) .$$

Equation (59) may be rewritten as

$$\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2}x_1 = \frac{1065 + 0.196(x_1+x_2)}{6} + (\frac{2}{3} + r_2)(C_p)_{f2}x_2$$

Hence r_2 is obtained as

$$r_2 = \frac{1065 + 0.196(x_1+x_2) + 4(C_p)_{f2}x_2 - 5(C_p)_{f1}x_1}{6(C_p)_{f2}(x_1-x_2)} . \qquad (60)$$

The value of Δt_2 is obtained by making an energy balance for the heat rejection section of the first effect. We can write

$$q_{1j} = F(1+r_i)(C_{p1})_{av}\,\Delta t_1$$

$$= F\{(C_p)_F + r_1(C_p)_{f1}\}\Delta t_1 .$$

We also have

$$q_{1j} = F\{(C_p)_F + r_2(C_p)_{f2}\}\Delta t_2 .$$

Hence

$$\Delta t_2 = \frac{(C_p)_F + r_1(C_p)_{f1}}{(C_p)_F + r_2(C_p)_{f2}}\,\Delta t_1 . \qquad (61)$$

The heat transfer area for the condenser tubes in the heat rejection section of the first effect, A_{1j}, is given by

$$A_{1j} = \frac{q_{1j}}{(U_1)_{av}\,(\Delta t)_{av1j}}$$

From equation (25) in the micro-stage model, we note that Δt_{av1j}, the average temperature difference for heat transfer, is

$$\Delta t_{av1j} = \frac{3(x_3^{20} - x_3^{23}) + 2(x_1^{20} - x_3^{20}) - 8}{6}$$

$$= \frac{3\Delta t_2 + 2(\Delta t_1 - 2) - 8}{6}$$

$$= \frac{3\Delta t_2 + 2\Delta t_1 - 12}{6}$$

The fixed charge cost for the condenser tubes of the heat rejection section of the first effect, $(x_4)_{1j}$, can thus be written as

$$(x_4)_{1j} = \frac{12C_3\{(C_p)_F + r_1(C_p)_{f1}\}\Delta t_1}{(U_1)_{av}(3\Delta t_2 + 2\Delta t_1 - 12)} \quad . \tag{62}$$

The rate of heat transfer for the condenser tubes of the heat recovery section of the second effect is

$$q_{2r} = F\{(\tfrac{5}{6} + r_2)(C_{p2})_{av} + \tfrac{1}{6}\}(x_1 - x_2 - \Delta t_2)$$

$$= F\{\tfrac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \tfrac{1}{6}\}(x_1 - x_2 - \Delta t_2) \quad .$$

For the condenser tubes the fixed charge cost $(x_4)_{c2}$ is

$$(x_4)_{c2} = \frac{C_3F[\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \frac{1}{6}](x_1 - x_2 - \Delta t_2)}{\frac{F}{2}(U_2)_{av}\left(\frac{41\Delta t_2 - x_1 + x_2 - 80}{40}\right)}$$

$$(x_4)_{c2} = \frac{80C_3[\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \frac{1}{6}](x_1 - x_2 - \Delta t_2)}{(U_2)_{av}(41\Delta t_2 - x_1 + x_2 - 80)} \quad . \tag{63}$$

The recycle cost for the second effect, $(x_4)_{r2}$ is (see equation (32) in the micro-stage model)

$$(x_4)_{r2} = \frac{2C_4 r_2 \times 144(P_1-P_2)}{62.5 \times 550 \times 3600 \times 0.85} \tag{64}$$

where

$$P_2 = \exp\left\{14.07 - \frac{9 \times 3660}{5(x_2 - 32) + 1989}\right\}$$

(C) Design Equations for the Third Effect. An energy balance for the third effect (refer to Fig. 12) gives

$$F(\tfrac{2}{3} + r_3)(C_{p3})_{av}x_2 = \tfrac{F}{6}(H_{v3})_{av} + F(\tfrac{1}{2} + r_3)(C_p)_{f3}x_3 \tag{65}$$

Since

$$(C_{p3})_{av} = \frac{\frac{2}{3}(C_p)_{f2} + r_3(C_p)_{f3}}{\frac{2}{3} + r_3}$$

and

$$(H_{v3})_{av} = 1065 + 0.196(x_2 + x_3),$$

equation (65) can be written as

$$\{\tfrac{2}{3}(C_p)_{f2} + r_3(C_p)_{f3}\}x_2 = \frac{1065+0.196(x_2+x_3)}{6} + (\tfrac{1}{2} + r_3)(C_p)_{f3}x_3$$

Solving for r_3, one obtains

$$r_3 = \frac{1065 + 0.196(x_2+x_3) + 3(C_p)_{f3}x_3 - 4(C_p)_{f2}x_2}{6(C_p)_{f3}(x_2 - x_3)} \tag{66}$$

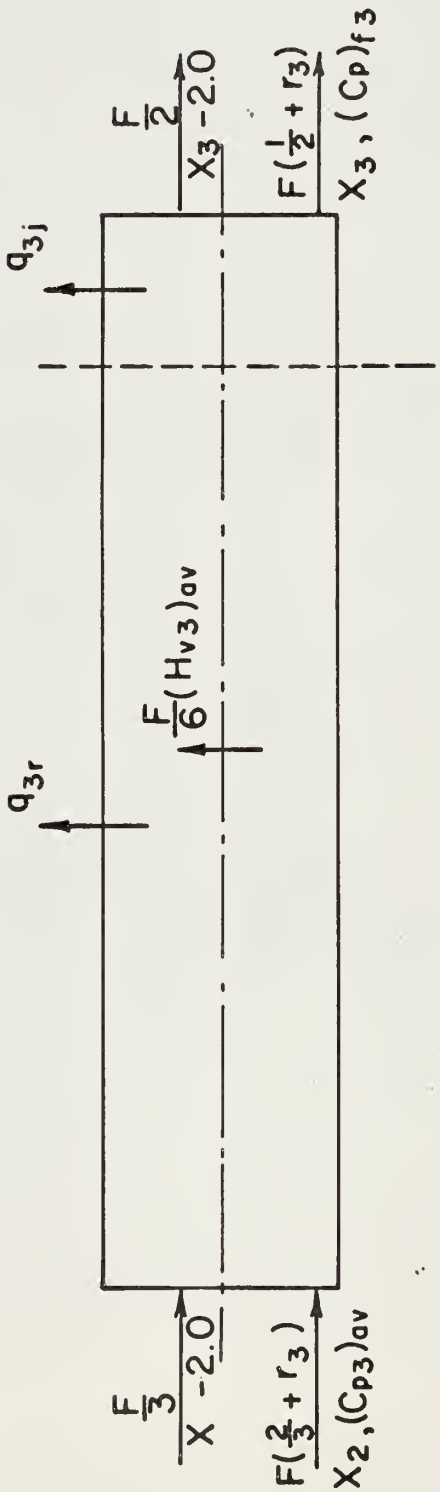


Fig. 12. Schematic flow diagram for the third effect.

The value of Δt_3 is obtained by making an energy balance around the heat rejection section of the second effect. One can write two equations

$$q_{2j} = F\left[\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \frac{1}{6}\right] \Delta t_2$$

$$q_{2j} = F\left[(C_p)_F + r_3(C_p)_{f3}\right] \Delta t_3$$

which when combined gives

$$\Delta t_3 = \frac{\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \frac{1}{6}}{(C_p)_F + r_3(C_p)_{f3}} \Delta t_2 \ . \tag{67}$$

The fixed charge cost for the condenser tubes of the heat rejection section of the second effect, $(x_4)_{2j}$, is

$$(x_4)_{2j} = \frac{12C_3\left\{\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \frac{1}{6}\right\} \Delta t_2}{(U_2)_{av}\,(3\Delta t_3 + 2\Delta t_2 - 12)} \ . \tag{68}$$

The rate of heat transfer for the condenser tubes of the heat recovery section of the third effect, q_{3r}, is

$$q_{3r} = F\left\{\left(\frac{2}{3} + r_3\right)(C_{p3})_{av} + \frac{1}{3}\right\}(x_2 - x_3 - \Delta t_3)$$

$$= F\left(\frac{2}{3}(C_p)_{f2} + r_3(C_p)_{f3} + \frac{1}{3}\right)(x_2 - x_3 - \Delta t_3)$$

The fixed charge cost, $(x_4)_{c3}$, is

$$(x_4)_{c3} = \frac{C_3 F\left(\frac{2}{3}(C_p)_{f2} + r_3(C_p)_{f3} + \frac{1}{3}\right)(x_2 - x_3 - \Delta t_3)}{\frac{F}{2}(U_3)_{av}\left(\frac{41\Delta t_3 - x_2 + x_3 - 80}{40}\right)}$$

$$(x_4)_{c3} = \frac{80C_3\left(\frac{2}{3}(C_p)_{f2} + r_3(C_p)_{f3} + \frac{1}{3}\right)(x_2 - x_3 - \Delta t_3)}{(U_3)_{av}(41\Delta t_3 - x_2 + x_3 - 80)} \tag{69}$$

The fixed charge cost for the condenser tubes of the heat rejection section of the third effect, $(x_4)_{3j}$, is

$$(x_4)_{3j} = \frac{8C_3\left\{\frac{2}{3}(C_p)_{f2} + r_3(C_p)_{f3} + \frac{1}{3}\right\}\Delta t_3}{(U_3)_{av}\left(\Delta t_3 + 2(x_3 - T_F) - 8\right)} \tag{70}$$

where from equation (47) in the microstage model, we see that

$$x_1^{66} + x_3^{66} - 2T_F - 6 = (x_1^{66} + 2 - x_3^{66}) + 2(x_3^{66} - T_F) - 6$$

$$= \Delta t_3 + 2(x_3 - T_F) - 8 .$$

Note that x_3 is the blowdown temperature of the third effect.

The recycle cost for the third effect, $(x_4)_{r3}$, is [see equation (44)]

$$(x_4)_{r3} = \frac{2C_4 r_3 \times 144(P_2 - P_3)}{62.5 \times 550 \times 3600 \times 0.85} \tag{71}$$

where

$$P_3 = \exp\left\{14.07 - \frac{9 \times 3660}{5(x_3 - 32) + 1989}\right\}$$

The dumping cost for the distillate and spent brine, $(x_4)_{DC}$, is [see equation (48) for the microstage model]

$$(x_4)_{DC} = \frac{2C_4 \times 144(14.7 - P_3)}{52.5 \times 550 \times 3600 \times 0.85} \tag{72}$$

The structure cost, $(x_4)_{Str}$, is [see equation (51) for the microstage model]

$$(x_4)_{Str} = \frac{43.2 \times 7.48 \times 24}{62.4 \times 5 \times 107} \tag{73}$$

The pumping cost for the make-up feed, $(x_4)_{FP}$, is [see equation (50) for the

micro-stage model]

$$(x_4)_{FP} = \frac{2C_4 \times 1.18\left\{(P_0 - 14.7)\frac{144}{62.5} + 50\right\}}{550 \times 3600} \qquad (74)$$

In summary, the total cost is the sum of the individual costs, which are

(1) the steam cost, equation (55)

(2) the fixed charge cost for the brine heater, equation (56)

(3) the fixed charge cost for the condenser tubes of each effect, equations (57), (62), (63), (68), (69), and (70).

(4) the recycle cost for each effect, equations (58), (64), and (71)

(5) the pumping cost for the make-up feed, equation (74)

(6) the pumping cost for the distillate and blowdown, equation (72)

(7) the structure cost, equation (73).

In addition to these costs, the general and administrative costs listed in Table 1 must be considered.

5. SIMULATION ACCORDING TO THE MACRO-STAGE MODEL

The simulation was carried out on the IBM 1620 computer. The design equations are listed in Table 8. The ranges of variables are shown in Table 9. The computer program symbols and computer program are put in Tables 10 and 11. The results are shown in Tables 12, 13 and 14.

6. DISCUSSION OF RESULTS

Comparison of results by both models are shown in Table 13. From this, we see that there is good agreement. The minor differences might be attributed to the temperature differences for heat transfer used for each case. It is also seen that the recycle ratios of each effect based on the amount of

TABLE 8

DESIGN EQUATIONS (THE MACROSTAGE MODEL)

Brine heater

(1) Steam Cost

$$\frac{2C_1\left\{(C_p)_F + r_1(C_p)_{f1}\right\}\Delta t_1}{\lambda_s} \qquad (55)$$

r_1 is calculated from

$$r_1 = \frac{1065 - 0.196(x_0+x_1) + 5(C_p)_{f1}x_1 - 6(C_p)_F x_0}{6(C_p)_{f1}(x_0 - x_1)} \qquad (54)$$

C_1 = given

λ_s = given

$(C_p)_F$, $(C_p)_{f1}$ given

Δt_1, x_0, x_1 assumed

(2) Fixed charge cost for the brine heater,

$$2C_2\left\{(C_p)_F + r_1(C_p)_{f1}\right\}\left\{\ln(24.4 + \Delta t_1) - \ln(24.4)\right\} \qquad (56)$$

C_2 = given

U_B = given

TABLE 8 (Cont'd)

The first effect — heat recovery section

(1) fixed charge cost for the condenser tubes

$$\frac{80C_3\left\{(C_p)_F + r_1(C_p)_{f1}\right\}(x_0 - x_1 - \Delta t_1)}{(U_1)_{av.}(41\Delta t_1 - x_0 + x_1 - 80)} \qquad (57)$$

C_3 : given

$(U_1)_{av.}$: given

(2) recycling cost

$$\frac{288\ C_4\ r_1(P_0 - P_1)}{62.5 \times 550 \times 3600 \times 0.85} \qquad (58)$$

C_4 : given

P_0 : given

P_1 is calculated from

$$P_1 = \exp\left(14.07 - \frac{9 \times 3660}{5(x_1 - 32) + 1989}\right),$$

The first effect — heat rejection section

$$\frac{12C_3\left\{(C_p)_F + r_1(C_p)_{F1}\right\}\Delta t_1}{(U_1)_{av.}(3\Delta t_2 + 2\Delta t_1 - 12)} \qquad (62)$$

Δt_2 is calculated from

$$r_2 = \frac{1065 + 0.196(x_1 + x_2) + 4(C_p)_{f2}x_2 - 5(C_p)_{f1}x_1}{6(C_p)_{f2}(x_1 - x_2)} \qquad (60)$$

TABLE 8 (Cont'd)

$$\Delta t_2 = \frac{(C_p)_F + r_1(C_p)_{f1}}{(C_p)_F + r_2(C_p)_{f2}} \Delta t_1 \qquad (61)$$

$(C_p)_{f2}$ = given,

x_2 = assumed,

The second effect — heat recovery section

(1) fixed charge cost for condenser tube,

$$\frac{80C_3\left(\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \frac{1}{6}\right)(x_1 - x_2 - \Delta t_2)}{(U_2)_{av.}(41\Delta t_2 - x_1 + x_2 - 80)} \qquad (63)$$

$(U_2)_{av.}$ = given

(2) recycling cost

$$\frac{288C_4\, r_2\, (P_1 - P_2)}{62.5 \times 550 \times 3600 \times 0.85} \qquad (64)$$

P_2 is calculated from,

$$P_2 = \exp\left(14.07 - \frac{9 \times 3660}{5(x_2 - 32) + 1989}\right)$$

The second effect — heat rejection section

(1) fixed charge cost for the condenser tube

$$\frac{12C_3\left(\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \frac{1}{6}\right)\Delta t_2}{(U_2)_{av.}(3\Delta t_3 + 2\Delta t_2 - 12)} \qquad (68)$$

Δt_3 is calculated from

$$r_3 = \frac{1065 + 0.196\,(x_2 + x_3) + 3(C_p)_{f3}x_3 - 4(C_p)_{f2}x_2}{6(C_p)_{f3}\,(x_2 - x_3)} \qquad (66)$$

TABLE 8 (Cont'd)

$$\Delta t_3 = \frac{\frac{5}{6}(C_p)_{f1} + r_2(C_p)_{f2} + \frac{1}{6}}{(C_p)_F + r_3(C_p)_{f3}} \Delta t_2 \qquad (67)$$

$(C_p)_{f3}$ = given

x_3 = assumed

The third effect — heat recovery section

(1) fixed charge cost for the condenser tube

$$\frac{80C_3\left(\frac{2}{3}(C_p)_{f2} + r_3(C_p)_{f3} + \frac{1}{3}\right)(x_2 - x_3 - \Delta t_3)}{(U_3)_{av.}(41\Delta t_3 - x_2 + x_3 - 80)} \qquad (69)$$

$(U_3)_{av.}$ = given

(2) recycle cost

$$\frac{288C_4 r_3 (P_2 - P_3)}{62.5 \times 550 \times 3600 \times 0.85} \qquad (71)$$

P_3 is calculated from

$$P_3 = \exp\left(14.07 - \frac{9 \times 3660}{5(x_3 - 32) + 1989}\right)$$

The third effect — heat rejection section

(1) fixed charge cost for the condenser tubes,

$$\frac{8C_3\left(\frac{2}{3}(C_p)_{f2} + r_3(C_p)_{f3} + \frac{1}{3}\right)\Delta t_3}{(U_3)_{av.}\left(\Delta t_3 + 2(x_3 - T_F) - 8\right)} \qquad (72)$$

T_F = given

TABLE 8 (Cont'd)

(2)	damping cost for the distillate and blowdown	$\frac{2 \times C_4 \times 144(14.7 - P_3)}{62.5 \times 550 \times 3600}$ P_3 = given (from steam table)	(72)
(3)	pumping cost for the make-up feed	$\frac{2\ C_4 1.18 \left\{ P_0 - 14.7)\frac{144}{62.5} + 50 \right\}}{550 \times 3600}$	(73)
(4)	construction cost	$\frac{43.2 \times 7.48 \times 24}{62.4 \times 5 \times 107}$	(74)

TABLE 9

RANGE OF VARIABLES

1.	Maximum temperature of flashing brine	(T_f) max < Ts (steam temperature)
2.	Minimum temperature of flashing	(T_f) min > T_F (temperature of make-up feed)
3.	intermediate blowdown temperature	(T_f) max > x_1, x_2 > (T_f) min
4.	total temperature difference between the flashing brine and recycle brine	$2 < \Delta t_n < 15$, n=1, 2, 3

In this section, we fix (T_f)max at 250°F and (T_f)min at 95.2～91.2°F. The intermediate temperatures are chosen such that the temperature interval is greater the previous one each time.

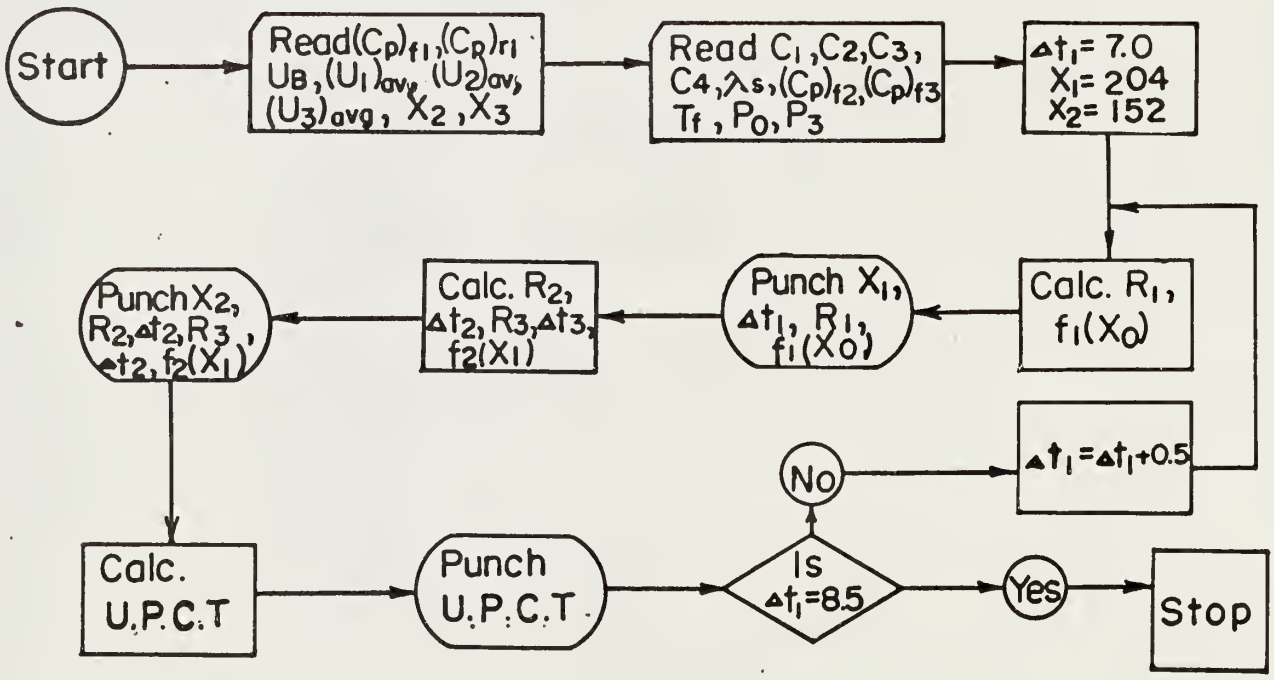


Fig. 13. Computer flow diagrame (the macro stage model).

TABLE 10

EXPLANATION OF PROGRAM SYMBOLS

(THE MACROSTAGE MODEL)

Symbol	Explanation
BHACT	fixed charge cost for the brine heater
C1	unit steam cost
C2	unit fixed charge cost for the brine heater
C3	unit fixed charge cost for the condenser tubes
C4	unit pumping cost
CPF	heat capacity of the make-up feed
CPF1	heat capacity of the flashing brine, the first effect
CPF2	heat capacity of the flashing brine, the second effect
CPF3	heat capacity of the flashing brine, the third effect
DCCT	pumping cost for the distillate and blowdown
DELT1	temperature rise through the brine heater
DELT2	temperature difference between the flashing and recycle brine, the second effect
DELT3	temperature difference between the flashing and recycle brine, the third effect
F1X0	unit production cost due to the first effect
F2X1	unit production cost due to the second and third effect
FBCT1	recycling cost, the first effect
FBCT2	recycling cost, the second effect
FBCT3	recycling cost, the third effect
FPCT	pumping cost for the make-up feed

TABLE 10 (Cont'd)

FT	temperature of make-up feed
PO	initial flashing pressure
P1	blowdown pressure, the first effect
P2	blowdown pressure, the second effect
P3	blowdown pressure, the third effect
R1	ratio of recycle brine in the first effect to the make-up feed
R2	ratio of recycle brine in the second effect to the make-up feed
R3	ratio of recycle brine in the third effect to the make-up feed
RMS	latent heat of steam
STMCT	steam cost
STRCT	structure cost
TAC1R	fixed charge cost for the condenser tubes, heat recovery section, the first effect
TAC1J	fixed charge cost for the condenser tubes, heat rejection section, the first effect
TAC2R	fixed charge cost for the condenser tubes, heat recovery section, the second effect
TAC2J	fixed charge cost for the condenser tubes, heat rejection section, the second effect
TAC3R	fixed charge cost for the condenser tubes, heat recovery section, the third effect
TAC3J	fixed charge cost for the condenser tubes, heat rejection section, the third effect
U1AV	average overall heat transfer coefficient of the condenser tubes, the first effect

TABLE 10 (Cont'd)

U2AV	average overall heat transfer coefficient of the condenser tubes, the second effect
U3AV	average overall heat transfer coefficient of the condenser tubes, the third effect
UB	overall heat transfer coefficient of the brine heater
UPCT	unit production cost
XO	maximum brine temperature
X1	blowdown temperature, the first effect
X2	blowdown temperature, the second effect
X3	blowdown temperature, the third effect

TABLE 11

SIMULATION OF THE MULTIFLASH EVAPOLATION PROCESS (THE MACROSTAGE MODEL)

```
   21 FORMAT(6X,6E10.4)
   51 FORMAT(1H 3F10.3,2X,E11.5)
   52 FORMAT(1H 5F10.3,2X,E10.4)
   53 FORMAT(1H E11.4)
      READ 21, CPF,CPF1,UB,U1AV,U2AV,U3AV
      READ 21,X0,C1,C2,C3,C4
      READ 21,RMS,CPF2,CPF3,FT,P0
      READ 21,DELT1,X1,X2,X3
      PRINT 21,CPF,CPF1,UB,U1AV,U2AV,U3AV
      PRINT 21,X0,C1,C2,C3,C4
      PRINT 21,RMS,CPF2,CPF3,FT,P0
      PRINT 21,DELT1,X1,X2,X3
C     CALC.F1X0
   12 R1=(1065.+.196*(X0+X1)+5.*CPF1*X1-6.*CPF*X0)/(6.*CPF1*(X0-X1))
      STMCT=2.*C1*(CPF+CPF1*R1)*DELT1/RMS
      BHACT=2.*C2*(CPF+CPF1*R1)*(LOG(24.4+DELT1)-LOG(24.4))/UB
      TAC1R=80.*C3*(CPF+CPF1*R1)*(X0-X1-DELT1)/U1AV/(41.*DELT1-X0+X1-
     180.)
      P1=EXP(14.07-9.*3660./(5.*(X1-32.)+1989.))
      FBCT1=2.*C4*R1*144.*(P0-P1)/62.5/550./3600./.85
      F1X0=STMCT+BHACT+TAC1R+FBCT1
      PUNCH 51,X1,DELT1,R1,F1X0
C     CALC.F2X1
      R2=(1065.+.196*(X1+X2)+4.*CPF2*X2-5.*CPF1*X1)/(6.*CPF2*(X1-X2))
      DELT2=(CPF+CPF1*R1)*DELT1/(CPF+CPF2*R2)
      R3=(1065.+.196*(X2+X3)+3.*CPF3*X3-4.*CPF2*X2)/(6.*CPF3*(X2-X3))
      DELT3=(5.*CPF1/6.+CPF2*R2+1./6.)*DELT2/(CPF+CPF3*R3)
      TAC1J=12.*C3*(CPF+CPF1*R1)*DELT1/U1AV/(3.*DELT2+2.*DELT1-12.)
      TAC2R=80.*C3*(5.*CPF1/6.+CPF2*R2+1./6.)*(X1-X2-DELT2)/U2AV/(41.*
     1DELT2-X1+X2-80.)
      TAC2J= 12.*C3*(5.*CPF1/6.+CPF2*R2+1./6.)*DELT2/U2AV/(3.*DELT3+
     12.*DELT2-12.)
      TAC3R=80.*C3*(2.*CPF2/3.+CPF3*R3+1./3.)*(X2-X3-DELT3)/U3AV/(41.
     1*DELT3-X2+X3-80.)
      TAC3J=8.*C3*(2.*CPF2/3.+CPF3*R3+1./3.)*DELT3/U3AV/(DELT3+2.*(X3
     1-FT)-8.)
```

```
( CONTINUED)
      P2=EXP(14.07-9.*3660./(5.*(X2-32.)+1989.))
      FBCT2=2.*C4*R2*144.*(P1-P2)/62.5/550./3600./.85
      P3=EXP(14.07-9.*3660./(5.*(X3-32.)+1989.))
      FBCT3=2.*C4*R3*144.*(P2-P3)/62.5/550./3600./.85
      DCCT=2.*C4*144.*(14.7-P3)/62.5/550./3600./.85
      FPCT=2.*C4*1.18*((P0-14.7)*144./62.5+50.)/550./3600.
      STRCT=43.2*7.48*24./(62.4*5.E7)
      F2X1=TAC1J+TAC2R+TAC2J+TAC3R+TAC3J+FBCT2+FBCT3+DCCT+FPCT+STRCT
      PUNCH 52,X2,R2,DELT2,R3,DELT3,F2X1
      UPCT=(F1X0+F2X1)*62.4*1.E3/7.48
      PUNCH 53,UPCT
      DELT1=DELT1+.05
      IF (DELT1-8.5) 12,12,15
   15 STOP
      END
      DATA
       .9650E 00 .9580E 00 .5371E 03 .5150E 03 .5100E 03 .5050E 03
       .2500E 03 .2500E-03 .3760E-04 .2397E-04 .6000E-02
       .9289E 03 .9475E 00 .9300E 00 .8500E 02 .2982E 02
       .6000E 01 .2060E 03 .1530E 03 .9400E 02
       .7000E 01 .2040E 03 .1520E 03 .9200E 02
       .8000E 01 .2020E 03 .1506E 03 .9520E 02
       .9000E 01 .2040E 03 .1520E 03 .9160E 02
       .1000E 02 .1980E 03 .1450E 03 .9000E 02
       .1200E 02 .1960E 03 .1460E 03 .9200E 02
       .1300E 02 .2040E 03 .1440E 03 .9250E 02
```

TABLE 12

SIMULATION RESULTS (THE MACROSTAGE MODEL)

Δt_1 °F	x_1 °F	x_2 °F	x_3 °F	r_1 lb/lb	r_2 lb/lb	r_3 lb/lb	Unit Cost $/10^3 gallon
8	202.0	150.6	95.2	2.441	2.523	2.613	0.2417
9	204.0	152.0	91.6	2.585	2.481	2.350	0.2453
6	206.0	153.0	94.0	2.742	2.417	2.417	0.2562
10	198.0	145.0	90.0	2.187	2.433	2.647	0.2457
12	196.0	146.0	92.0	2.074	2.626	2.604	0.2541
13	204.0	144.0	91.5	2.585	2.057	2.866	0.2833

TABLE 13

COMPARISON OF RESULTS

THE MACROSTAGE MODEL

Δt_1 °F	x_1 °F	x_2 °F	x_3 °F	r_1 lb/lb	r_2 lb/lb	r_3 lb/lb	Unit Cost $/10^3 gallon
8	202.0	150.6	95.2	2.441	2.523	2.613	0.2417
9	204.0	152.0	91.6	2.585	2.481	2.350	0.2453

THE MICROSTAGE MODEL

Δt_1 °F	$(T_f)_{23}$ °F	$(T_f)_{46}$ °F	$(T_f)_{68}$ °F	r_1 lb/lb	r_2 lb/lb	r_3 lb/lb	Unit Cost $/10^3 gallon
8	201.967	150.638	95.214	2.54	2.60	2.66	0.2491
9	203.972	150.962	91.588	2.69	2.48	2.43	0.2511

make-up feed according to the macrostage model are lower than those by the microstage model. The macrostage model also gave lower unit production costs.

As we mentioned in Section 1, the cost figures calculated are only the sum of the in-plant operation and capital charge costs. Additional cost items listed in Table 1 should be incorporated to make up the unit production cost, and thus the unit production cost becomes 0.42 ~0.43 $ per 1000 gallons. According to Ref. (3) the best unit production cost reported for a plant of 50 MM gallon per day with a single effect multistage model is 0.449 $ per 1000 gallons. The cost difference might be due to the thermodynamic advantage of the multieffect multistage model; however, we did not calculate the cost due to friction losses in the condenser tubes and channels. These are known to be of minor importance in the evaluation of cost functions.

The simulation results by varying Δt_1 in the range of 7.0 ~ 8.0°F with fixed values for $x_1 = 204^{\circ}F$, $x_2 = 152^{\circ}F$, $x_3 = 92^{\circ}F$ according to the macrostage model are shown in Table 14.

TABLE 14

CALCULATION RESULTS BY THE MACROSTAGE MODEL

$x_1=204^oF$ $x_2=152^oF$ $x_3=92^oF$

Δt_1 ^oF	r_1 lb/lb	$f_1(x_0)$ \$/lb x 10^{-5}	r_2 lb/lb	Δt_2 ^oF	r_3 lb/lb	Δt_3 ^oF	$f_2(x_1)$ \$/lb x 10^{-5}	Unit Cost \$/10^3 gallon
7.00	2.585	1.694	2.481	7.264	2.369	7.603	1.244	0.24511
7.05	2.585	1.699	2.481	7.316	2.369	7.657	1.234	0.24472
7.10	2.585	1.704	2.481	7.368	2.369	7.711	1.225	0.24436
7.15	2.585	1.709	2.481	7.420	2.369	7.765	1.215	0.24403
7.20	2.585	1.715	2.481	7.472	2.369	7.820	1.206	0.24373
7.25	2.585	1.720	2.481	7.524	2.369	7.864	1.198	0.24345
7.30	2.585	1.726	2.481	7.575	2.369	7.928	1.189	0.24320
7.35	2.585	1.731	2.481	7.627	2.369	7.983	1.181	0.24298
7.40	2.585	1.737	2.481	7.679	2.369	8.037	1.163	0.24277
7.45	2.585	1.743	2.481	7.731	2.369	8.091	1.165	0.24259
7.50	2.585	1.649	2.481	7.783	2.369	8.146	1.157	0.24243
7.55	2.585	1.755	2.481	7.835	2.369	8.200	1.149	0.24230
7.60	2.585	1.761	2.481	7.886	2.369	8.254	1.142	0.24218
7.65	2.585	1.767	2.481	7.939	2.369	8.309	1.135	0.24208
7.70	2.585	1.773	2.481	7.991	2.369	8.363	1.127	0.24200
7.75	2.585	1.779	2.481	8.042	2.369	8.417	1.120	0.24194
7.80	2.585	1.786	2.481	8.094	2.369	8.471	1.114	0.24190
7.85	2.585	1.792	2.481	8.146	2.369	8.526	1.107	0.24188
7.90	2.585	1.798	2.481	8.198	2.369	8.580	1.101	0.24187
7.95	2.585	1.805	2.481	8.250	2.369	8.634	1.094	0.24188
8.00	2.585	1.811	2.481	8.302	2.369	8.689	1.088	0.24191

TABLE 14 (Cont'd)

Δt_1	r_1	$f_1(x_0)$	r_2	Δt_2	r_3	Δt_3	$f_2(x_1)$	Unit Cost
^oF	lb/lb	\$/lb x 10^{-5}	lb/lb	^oF	lb/lb	^oF	\$/lb x 10^{-5}	\$/10^3 gallon
8.05	2.585	1.818	2.481	8.354	2.369	8.743	1.082	0.24195
8.10	2.585	1.825	2.481	8.406	2.369	8.796	1.076	0.24200
8.15	2.585	1.831	2.481	8.458	2.369	8.852	1.080	0.24292
8.20	2.585	1.838	2.481	8.509	2.369	8.906	1.064	0.24216
8.25	2.585	1.845	2.481	8.561	2.369	8.960	1.059	0.24226
8.30	2.585	1.852	2.481	8.613	2.369	9.015	1.053	0.24236
8.35	2.585	1.866	2.481	8.716	2.369	9.069	1.048	0.24249
8.40	2.585	1.866	2.481	8.717	2.369	9.123	1.042	0.24263
8.45	2.585	1.873	2.481	8.769	2.369	9.177	1.037	0.24278
8.50	2.585	1.880	2.481	8.821	2.369	9.232	1.032	0.24294

References

1. Saline Water Conversion Report, 1964, United States Department of the Interior, Office of Saline Water, "Multieffect Multistage (MEMS) Flash Distillation Process," 1964.

2. The Fluor Corporation, "Computational Design Study on 50 Million Gallon per day MSM Desalination Plant for Office of Saline Water, U.S. Department of the Interior," Final Report, Jan. 1965.

3. Bechtel Corporation, "Cost Studies of Large Multi-stage Flash Saline Water Conversion Plants for Office of Saline Water," Research and Development Progress Report No. 116, Oct. 1964.

4. Hala, E., et al., "Vapor-liquid Equilibrium," Pergamon Press, New York, 1958.

APPENDIX II

OPTIMIZATION OF THE MULTI-EFFECT, MULTI-STAGE EVAPORATION PROCESS BY THE MAXIMUM PRINCIPLE

We shall employ the design equations obtained by the macro-stage model in Appendix I to carry out the optimization of the multiflash evaporation process by means of a discrete form of the maximum principle [1]. The reason we use this model is that it is simpler in its form than the micro-stage model. Since we assumed equal temperature drops for the flashing brine in each stage and also that the temperature differences between the flashing brine and the recycle brine are equal all the way through the heat recovery section of each effect, we can treat the process as a stage-wise one-dimensional decision process and apply the discrete maximum principle, to optimize it. In the formulation of the discrete maximum principle we choose the temperatures of the flashing brine at the exit of each effect as state variables and the ratios of the recycle brine in each effect to the make up feed as decision variables. The optimization problem is defined so that the first stage is the combination of the brine heater and the heat recovery section of the first effect, the second stage is just the heat recovery section of the second effect, and the third stage is the third effect itself. The reason why the heat rejection sections of the first two effects are excluded is that they involve two different Δt's of the adjacent effects. This leads to a "process with decisions in memory" [1] in evaluating the cost equations. However, by excluding these two sections from our optimization study, the problem is reduced to the standard type without memory.

1. STATEMENT OF THE PROBLEM

It should be noted that equal distillate production is assumed for each effect in this formulation. Then it follows that the blowdown concentrations are

$$(C_f)_{1b} = 0.042,$$

$$(C_f)_{2b} = 0.0525,$$

$$(C_f)_{3b} = 0.07.$$

The heat capacities of the flashing brine corresponding to these concentrations are

$$(C_p)_{f1} = 0.958,$$

$$(C_p)_{f2} = 0.9475,$$

$$(C_p)_{f3} = 0.93.$$

An energy balance around the brine heater and first effect (see Fig. 1) gives

$$q + F(C_p)_f tr_2 + Fr_2(C_p)_{r2} tr_2 = \frac{F}{6}(x_1 - \Delta t_{BPE}) + (\frac{5}{6} + r_2)F(C_{p2})_{av} x_1 \qquad (1)$$

where $x_1 = t_f$

$$q + F(1+r_2)(C_{p2})_{av} tr_2 = F(1+r_2)(C_{p2})_{av} x_1$$

Solving for $\Delta t_2 = x_1 - tr_2$, we obtain

$$\Delta t_2 = x_1 - tr_2 = \frac{q}{F(1+r_2)(C_{p2})_{av}} \qquad (2)$$

In the same manner it can be shown that

$$\Delta t_3 = \frac{q}{F(1+r_3)(C_{p3})_{av}} \qquad (3)$$

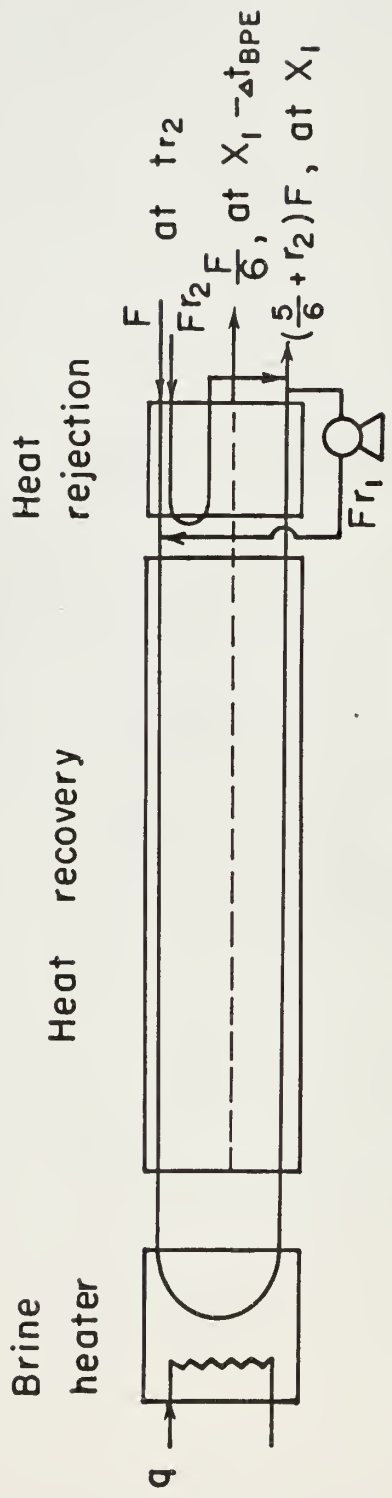


Fig. 1. A block diagram for the first effect.

and that

$$\Delta t_1 = \frac{q}{F(1+r_1)(Cp_1)_{av}} \tag{4}$$

Since, the magnitudes of the recycle ratios are known from the previous simulation, we can assign approximate values to the average heat capacities without knowing the exact values of the recycle ratio

$$(Cp_1)_{av} = 0.96,$$

$$(Cp_2)_{av} = 0.952,$$

$$(Cp_3)_{av} = 0.94.$$

Note that equations (2), (3), and (4) all contain the factor $\frac{q}{F}$, and for this reason we will choose $\frac{q}{F}$ as a parameter in our optimization study.

2. OPTIMAL SOLUTION BY THE DISCRETE MAXIMUM PRINCIPLE

According to the algorithm of the discrete maximum principle [1], we define the temperature of the flashing brine as the state variable x_1 with a transformation equation at each stage of the form

$$x_1^n = T^n (x_1^{n-1}; \theta^n)^*$$

where θ^n is the recycle ratio which is the decision to be made at each stage. Using the notation introduced here, equation (54) in Appendix I becomes

$$\theta^1 = \frac{1065 + 0.196(x_1^0 + x_1^1) + 5 \times 0.958x_1^1 - 6 \times 0.965x_1^0}{6 \times 0.958 (x_1^0 - x_1^1)} \tag{5}$$

---

*All superscripts stand for the stage number.

Solving this equation for x_1^1 gives

$$x_1^1 = T^1(x_1^0; \theta^1) = \frac{(5.748\ \theta^1 + 5.594)x_1^0 - 1065}{5.748\ \theta^1 + 4.986} \tag{6}$$

Similarly, equation (60) becomes

$$\theta^2 = \frac{1065 + 0.196(x_1^1 + x_1^2) + 4 \times 0.9475x_1^2 - 5 \times 0.958x_1^1}{6 \times 0.9475(x_1^1 - x_1^2)} \tag{7}$$

which may be rewritten as

$$x_1^2 = T^2(x_1^1; \theta^2) = \frac{(5.685\ \theta^2 + 4.594)x_1^1 - 1065}{5.685\ \theta^2 + 3.986} \tag{8}$$

From equation (66), we can obtain

$$\theta^3 = \frac{1065 + 0.196(x_1^2 + x_1^3) + 3 \times 0.93x_1^3 - 4 \times 0.9475x_1^2}{6 \times 0.93(x_1^2 - x_1^3)} \tag{9}$$

by introducing the new notation. Solving equation (9) for x_1^3 gives

$$x_1^3 = T^3(x_1^2, \theta^3) = \frac{(5.58\ \theta^3 + 3.594)x_1^2 - 1065}{5.58\ \theta^3 + 2.986} \tag{10}$$

We shall introduce a new state variable x_2 for the accumulated unit production cost. We shall show that the accumulated unit production cost can be written in the form

$$x_2^n = x_2^{n-1} + G^n(x_1^{n-1}; \theta^n),\ x_2^0 = 0 \quad n = 1, 2, 3. \tag{11}$$

It is obvious that $\sum_{n=1}^{3} G^n(x_1^{n-1};\ \theta^n) = x_2^3$. Thus the problem is transformed into the standard form in which a sequence of θ^n, n = 1, 2, 3 is to be chosen so as to minimize the objective function x_2^3 for a process described by equations (6), (8), and (10).

The terms which comprise the cost functions, $G^n(x_1^{n-1};\ \theta^n)$, n = 1, 2, 3, have been derived in Appendix I. In this optimization study, $G^1(x_1^0;\ \theta^1)$ is comprised of the steam cost, the fixed charge cost for the brine heater, and the fixed charge cost for the condenser tubes of the heat recovery section of the first effect. The steam cost is obtained from equation (55) of Appendix I as

$$(x_4)_s = \frac{2C_1 q}{F\lambda_s} \tag{12}$$

The fixed charge cost for the brine heater is obtained by rewriting equation (56) as

$$(x_4)_B = \frac{1.92C_2(1+\theta^1)}{U_B}\left\{\ln\left(24.4 + \frac{q}{0.96F(1+\theta^1)}\right) - \ln(24.4)\right\} \tag{13}$$

The fixed charge cost for the condenser tubes of the heat recovery section of the first effect is obtained by substituting equation (6) into equation (57). This gives

$$(x_4)_{c1} = \frac{80C_3(1+\theta^1)0.96\left\{x_1^0 - \dfrac{(5.748\theta^1 + 5.594)x_1^0 - 1065}{5.748\theta^1 + 4.986} - \dfrac{q}{F(1+\theta^1)0.96}\right\}}{(U_1)_{av}\left\{\dfrac{41q}{F(1+\theta^1)0.96} - x_1^0 + \dfrac{(5.748\ \theta^1 + 5.594)x_1^0 - 1065}{5.748\ \theta^1 + 4.986} - 80\right\}}$$

$$= \frac{80C_3 \times 0.96(1+\theta^1)\left\{\dfrac{1065 - 0.608\, x_1^0}{5.748\,\theta^1 + 4.986} - \dfrac{q}{F(1+\theta^1)0.96}\right\}}{(U_1)_{av}\left\{\dfrac{41q}{F(1+\theta^1)0.96} - \dfrac{1065 - 0.608\, x_1^0}{5.748\,\theta^1 + 4.986} - 80\right\}}$$

$$= \frac{76.8C_3(1+\theta^1)\left\{0.96(1+\theta^1)(1065 - 0.608x_1^0 - \frac{q}{F}(5.748\theta^1 + 4.986)\right\}}{(U_1)_{av}\left\{\frac{41q}{F}(5.748\theta^1+4.986) - 0.96(1+\theta^1)(1463.9-0.608x_1^0+459.8\theta^1)\right\}} \quad (14)$$

We will not include the recycle cost in this optimization study because the total recycle cost itself is small compared to the total production cost. In addition to this, the pressure

$$\Delta P_{total} = (P_0 - P_1) + (P_1 - P_2) + (P_2 - P_3)$$

$$= \Delta P_1 + \Delta P_2 + \Delta P_3$$

is almost constant since the total temperature range of the flashing process can only be varied a few degrees Fahrenheit. Thus, an increase in one ΔP will decrease the other two ΔPs. It is also intuitively seen that the recycle cost for each effect itself cannot vary much.

As mentioned earlier, the production cost due to the fixed charge costs for the condenser tubes in the heat rejection sections of the first and the second effects are excluded from our consideration. Since there are only 6 of the 68 stages in these sections the optimal unit production cost will not be influenced very much in case they are not taken into account. Since they involve decisions in memory as will be shown below, they complicate the optimization problem.

Rewriting equation (62) in Appendix I for the fixed charge cost for the condenser tubes in the heat rejection section of the first effect we have

after substituting equations (2) and (4) into equation (62)

$$(x_4)_{1j} = \frac{12C_3 \frac{q}{F}}{(U_1)_{av}\left\{\frac{3q}{F(1+\theta^2)0.952} + \frac{2q}{F(1+\theta^1)0.96} - 12\right\}}$$

$$(x_4)_{1j} = \frac{12C_3}{(U_1)_{av}\left\{\frac{3}{0.952(1+\theta^2)} + \frac{2}{0.96(1+\theta^1)} - \frac{12F}{q}\right\}} \qquad (15)$$

A similar expression can be obtained for the heat rejection section of the second effect by substituting equations (2) and (3) into equation (68) of Appendix I. One obtains

$$(x_4)_{2j} = \frac{12C_3}{(U_2)_{av}\left\{\frac{3}{0.94(1+\theta^3)} + \frac{2}{0.952(1+\theta^2)} - \frac{12F}{q}\right\}} \qquad (16)$$

Equations (15) and (16) each contain two decision variables and because of this they can't be included in cost functions of the form $G^n(x_1^{n-1}; \theta^n)$. In order to include equations (15) and (16) a new state variable would have to be introduced (1). However, in this study equations (15) and (16) will be added in after the optimal solution has been found.

From equations (12), (13), and (14) we thus obtain

$$G^1(x_1^0; \theta^1) = (x_4)_s + (x_4)_B + (x_4)_{cl} \qquad (17)$$

In this optimization study, $G^2(x_1^1; \theta^2)$ is the fixed charge cost for the condenser tubes in the heat recovery section of the second effect. Substituting equations (2) and (8) into equation (63) in Appendix I we obtain

$$G^2(x_1^1;\ \theta^2) = \frac{80C_3(1+\theta^2)0.952\left\{x_1^1 - \dfrac{(5.685\ \theta^2 + 4.594)\ x_1^1 - 1065}{5.685\ \theta^2 + 3.986} - \dfrac{q}{F(1+\theta^2)0.952}\right\}}{(U_2)_{av}\left\{\dfrac{q}{F(1+\theta^2)0.952} - x_1^1 + \dfrac{(5.685\ \theta^2 + 4.594)x_1^1 - 1065}{5.685\ \theta^2 + 3.986} - 80\right\}}$$

which can be simplified to give

$$G^2(x_1^1;\ \theta^2) = \frac{76.16C_3(1+\theta^2)\left\{0.952(1+\theta^2)(1065-0.608x_1^1) - \frac{q}{F}(5.685\theta^2+3.986)\right\}}{(U_2)_{av}\left\{\frac{41q}{F}(5.685\theta^2+3.986) - 0.952(1+\theta^2)(1383.9-0.608x_1^1+454.8\theta^2)\right\}} \quad (18)$$

$G^3(x_1^2;\ \theta^3)$ represents the fixed charge cost for the condenser tubes in both the heat recovery and heat rejection sections of the third effect. From equation (69) in Appendix I, the fixed charge cost for the condenser tubes in the heat recovery section of third effect is obtained by substituting equations (3) and (10) for x_1^3 and Δt_3

$$(x_4)_{c3} = \frac{80C_3(1 + \theta^3)0.94\left\{x_1^2 - \dfrac{5.58\ \theta^3 + 3.594)x_1^2 - 1065}{5.58\ \theta^3 + 2.986} - \dfrac{q}{F(1 + \theta^3)0.94}\right\}}{(U_3)_{av}\left\{\dfrac{41q}{F(1 + \theta^3)0.94} - x_1^2 + \dfrac{(5.58\ \theta^3 + 3.594)x_1^2 - 1065}{5.58\ \theta^3 + 2.986} - 80\right\}}$$

On simplification, it becomes

$$(x_4)_{c3} = \frac{75.2C_3(1+\theta^3)\left\{0.94(1+\theta^3)(1065-0.608x_1^2) - \frac{q}{F}(5.58\theta^3+2.986)\right\}}{(U_3)_{av}\left\{\frac{41q}{F}(5.58\theta^3+2.986) - 0.94(1+\theta^3)(1303.9-0.608x_1^2+446.4\theta^3)\right\}} \quad (19)$$

By substituting equations (3) and (10) into equation (70) in Appendix 1, the fixed charge cost for the condenser tubes in the heat rejection section of the third effect is obtained as

$$(x_4)_{3j} = \frac{8C_3(1+\theta^3)0.94\,\dfrac{q}{F(1+\theta^3)0.94}}{(U_3)_{av}\left\{\dfrac{q}{F(1+\theta^3)0.94} + \dfrac{2\{(5.58\,\theta^3 + 3.594(x_1^2 - 1065\}}{5.58\,\theta^3 + 2.986} - (2T_F + 8)\right\}}$$

$$= \frac{8C_3}{(U_3)_{av}\left\{\dfrac{1}{0.94(1+\theta^3)} + \dfrac{2F\{15.8\,\theta^3 + 3.594)x_1^2 - 1065\}}{q(5.58\,\theta^3 + 2.986} - \dfrac{F(2T_F + 8)}{q}\right\}}.$$

On further simplification, it becomes

$$\frac{7.52C_3(1+\theta^3)(5.58\,\theta^3 + 2.986)}{(U_3)_{av}\left[(5.58\,\theta^3 + 2.986) + \dfrac{3F}{q}\{(5.58\,\theta^3 + 3.594)\,x_1^2 - 1065\}0.94(1+\theta^3)\right.}$$

$$\left. - 0.94(1+\theta^3)\,\frac{F}{q}\,(2T_F + 8)(5.58\,\theta^3 - 2.986)\right]$$

Thus, we can write

$$G^3(x_1^2;\ \theta^3 = (x_4)_{c3} + (x_4)_{3j}$$

Now we observe that our cost equations have the standard form of the discrete maximum principle.

$$x_2^0 = 0$$

$$x_2^1 = x_2^0 + G^1(x_1^0;\ \theta^1),$$

$$x_2^2 = x_2^1 + G^2(x_1^1;\ \theta^2),$$

$$x_2^3 = x_2^2 + G^3(x_1^2;\ \theta^3),$$

and

$$\text{Min. } S = \text{Min. } \sum_{n=1}^{3} G^n(x_1^{n-1};\ \theta^n) = \text{Min. } x_2^3$$

A block diagram for the process is shown in Fig. 2.

The procedure for solving such an optimization problem by the discrete maximum principle is to introduce adjoint vectors z^n and Hamiltonian functions H^n such that

$$H^n = \sum_{i=1}^{2} z_i^n x_i^n \qquad n = 1, 2, 3,$$

$$z_i^{n-1} = \frac{\partial H^n}{\partial x_i^{n-1}}, \qquad n = 1, 2, 3,; \quad i = 1, 2.$$

Then,

$$H^1 = z_1^1 x_1^1 + z_2^1 x_2^1 = z_1^1 x_1^1 + z_2^1 G^1(x_1^0; \theta^1)$$

$$H^2 = z_1^2 x_1^2 + z_2^2 x_2^2 = z_1^2 x_1^2 + z_2^2\{x_2^1 + G^2(x_1^1; \theta^2)\}$$

$$H^3 = z_1^3 x_1^3 + z_2^3 x_2^3 = z_1^3 x_1^3 + z_2^3\{x_2^2 + G^3(x_1^2; \theta^3)\}$$

It is obvious that

$$z_2^1 = \frac{\partial H^2}{\partial x_2^1} = z_2^2 = \frac{\partial H^3}{\partial x_2^2} = z_2^3 = 1,$$

$$z_1^3 = 0,$$

Hence, we can write

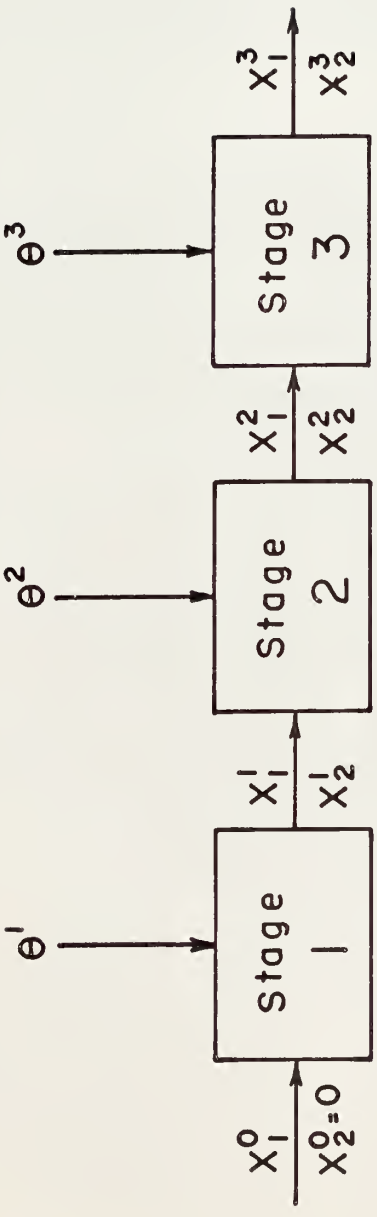


Fig. 2. A block diagram for the multiflash evaporation process.

$$H^1 = z_1^1 x_1^1 + x_2^1 = z_1^1 \left\{ \frac{(5.748\,\theta^1 + 5.594)x_1^0 - 1065}{5.748\,\theta^1 + 4.986} \right\} + \frac{2C_1 q}{F\lambda_s}$$

$$+ \frac{1.92C_2(1 + \theta^1)}{U_B} \left\{ \ln\left(24.4 + \frac{q}{0.96F(1 + \theta^1)}\right) - \ln(24.4) \right\}$$

$$+ \frac{76.8C_3(1+\theta^1)\left\{0.96(1+\theta^1)(1065-0.608x_1^0) - \frac{q}{F}(5.748\theta^1+4.986)\right\}}{(U_1)_{av}\left\{\frac{41q}{F}(5.748\theta^1+4.986) - 0.96(1+\theta^1)(1463.9-0.608x_i^0+459.8\theta^1)\right\}} \quad (21)$$

$$H^2 = z_1^2 x_1^2 + x_2^1 + G^2(x_1^1;\ \theta^2) = z_1^2 \left\{ \frac{(5.685\,\theta^2 + 4.594)x_1^1 - 1065}{5.685\,\theta^2 + 3.986} \right\}$$

$$+ x_2^1 + \frac{76.16C_3(1+\theta^2)\left\{0.952(1+\theta^2)(1065-0.608x_1^1) - \frac{q}{F}(5.685\theta^2+3.986)\right\}}{(U_2)_{av}\left\{\frac{41q}{F}(5.685\theta^2+3.986)-0.952(1+\theta^2)(1383.9-0.608x_1^1+454.8\theta^2)\right\}} \quad (22)$$

$$H^3 = z_1^3 x_1^3 + x_2^2 + G^3(x_1^2;\ \theta^3) = z_1^3 \left\{ \frac{5.58\,\theta^3 + 3.594)x_1^2 - 1065}{5.58\,\theta^3 + 2.986} \right\}$$

$$+ x_2^2 + \frac{75.2C_3(1+\theta^3)\left\{0.94(1+\theta^3)(1065-0.608x_1^2) - \frac{q}{F}(5.58\theta^3+2.986)\right\}}{(U_3)_{av}\left\{\frac{41q}{F}(5.58\theta^3+2.986)-0.94(1+\theta^3)(1303.9-0.608x_1^2+446.4\theta^3)\right\}}$$

$$+ \frac{7.52C_3(1 + \theta^3)(5.58\,\theta^3 + 2.986)}{(U_3)_{av}\left\{(5.58\theta^3+2.986) + \frac{2F}{q}\left\{(5.58\theta^3+3.594)x_1^2-1065\right\}0.94(1+\theta^3) - \right.}$$

$$\left. \frac{}{0.94\,\frac{F}{q}\,(1 + \theta^3)2T_F + 8)(5.58\,\theta^3 - 2.986)\right\}} \quad (23)$$

3. COMPUTATIONAL SCHEME

A computational procedure which might be used to obtain the optimal values for the process, if the decision variable is not constrained or the optimal value is in the interior of the admissible range of the decision variable, is as follows:

1. Assume a value for x_1^3

2. Differentiate equation (23) to obtain $\frac{\partial H^3}{\partial \theta^3}$. If the decision variable is not constrained, we must have $\frac{\partial H^3}{\partial \theta^3} = 0$ (24)

3. Determine x_1^2 and θ^3 by solving equations (10) and (24) simultaneously. This might be done by assuming an initial value for θ^3, finding x_1^2 from equation (10), evaluating $\frac{\partial H^3}{\partial \theta^3}$, and then using the method of steepest descent in the form

$$\theta^3_{new} = \theta^3_{old} - K\frac{\partial H^3}{\partial \theta^3}\Big|\theta^3_{old}$$

to find a better value of θ^3.

4. Evaluate $z_1^2 = \frac{\partial H^3}{\partial x_1^2}$ using the obtained values of x_1^2 and θ^3 and substitute it into equation (22).

5. Use the $\frac{\partial H^2}{\partial \theta^2} = 0$, relation (25)

and equation (8) to determine x_1^1 and θ^2 by solving these equations simultaneously as in step 3.

6. Evaluate $z_1^1 = \frac{\partial H^2}{\partial x_1^1}$ for the obtained values of x_1^1 and θ^2; and substitute

it into equation (21),

7. Use equation (6) and the relation $\frac{\partial H^1}{\partial \theta^1} = 0$ (26)

to determine x_1^0 and θ^1 by solving these equations simultaneously as in step (3),

8. Compare the computed value of x_1^0 with the given value of x_1^0. The above procedure is repeated until the calculated value of x_1^0 is approximately equal to the given value.

It is recalled that the plant we are considering has the capacity of 50 MM gallons of distillate per day so that every cost item should be based on this capacity.

In Ref. (2) and Ref. (3) the values q/F = 20.6 and 33.7, respectively were used. The system under investigation here is closer to the case given in Ref. (2). Based on these previous studies a reasonable range of the parameter, q/F, and the decision variables to be used in the computation is

1) $q/F = 22\sim28$

2) $\theta^n = 2.0\sim2.6.$

The range of the decision variables is taken intuitively from the simulation results and review of Ref. (2).

In principle, smaller values of θ^n are desired.

Because

$$\Delta t^n = \frac{q}{F(1 + \theta^n)(C_{pn})_{av}}$$

If $\frac{q}{F}$ is given, we can see that the smaller the values of θ^n, the larger the value of Δt^n, and thus less condenser tube area is needed for each effect so that the production cost is reduced. But θ^n can't be too

small because a certain amount of recycle brine is needed for each effect in order to increase the heat capacity of the flashing brine stream so that for a given production of distillate the total temperature drop of the flashing brine satisfies the conditions

3) $x_1^0 = 250^\circ F$

$x_1^3 = 90 \sim 95^\circ F$

The maximum brine temperature x_1^0 is fixed at about $250^\circ F$ from the point of view of scale-formation. The blowdown temperature cannot be too high or too low. In case it is too high, heat waste becomes appreciable and in case it is too low, the condenser tube area in the heat rejection section and the pumping cost for the coolant increase. In view of this the blowdown temperature x_1^3 should be taken as $90 \sim 95^\circ F$ in this study.

It is also noted that the computational procedure stated earlier is only valid for the case in which the optimal decision is interior to the set of admissible decisions. If the optimal decision lies on the boundary of the set the necessary condition for x_2^3 to be a minimum is

$$H^n = \text{minimum}$$

where n denotes only those stages where the optimal decision lies on the boundary of the set.

REFERENCES

1. Fan, L. T. and Wang, C. S. "The Discrete Maximum Principle," John Wiley & Sons, New York, 1964

2. The Fluor Corporation "Computational Design Study on 50 Million gallon per day MSM desalination plant for office of Saline water, U.S. Department of the Interior" Final Report Jan. 1965

3. Bechtel Corporation "Cost Studies of Large Multi-Stage Flash Saline Water Conversion Plants for Office of Saline Water" Research and Development Progress Report No. 116. Oct. 1964.

APPLICATIONS OF DYNAMIC PROGRAMMING TO PROCESS ENGINEERING

by

LIEN-CHENG SU

B. S., National Taiwan University, 1955

AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1967

This work shows how the method of dynamic programming can be used to optimize chemical processing systems by treating several examples.

The principle of optimality and the functional equation which constitutes the basic algorithm of the method of dynamic programming are presented. The computational scheme for the functional equation and the table entry procedure are given in detail followed by some simple examples. The optimal allocation of back-mix reactor volumes for a two phase, second order reaction system is considered for both countercurrent and co-current flow. The results show that the countercurrent flow scheme is more economical than the co-current flow scheme especially at higher conversions.

The optimization of a multieffect, multistage evaporator system with a nominal capacity of 20 MM gallons per day of distillate is considered. Using the cost estimating procedures recommended by the Office of Saline Water, an optimal unit production cost of 40¢ per 1000 gallons was obtained. This particular study serves to illustrate the applicability of dynamic programming to the optimization of a multistage decision process whose first appearance seems to be complex.

The refinement of solutions and the reduction in dimensionality are discussed. Since the discretization errors are inherent with the method of dynamic programming, one or another method of interpolation or extrapolation should be used to refine the solutions. Furthermore, the methods that can be used to obtain a reduction in dimensionality are described fully because of the exponential increase in computer memory that occurs with an increase in the number of state variables. Often the successful application of the dynamic programming technique is obstructed by the dimensionality problem. The k-th best policy is also given to illustrate how to find suboptimal

policies which are the best alternatives to the optimal policy. The application of the k-th best method is illustrated by several simple examples and the optimization of a multistage decision process with parallel redundancy. The optimization procedure for treating complex multistage decision processes is also given and some examples are treated in order to illustrate the technique for optimizing nonsequential, geometrically complex processes.

The transformation and cost equations for both a microstage and a macrostage model of a multieffect, multistage flash evaporation system are developed and compared. Due to the simplicity of the macrostage model, the design equations for the macrostage model are used for the dynamic programming optimization. Results of simulation studies which were made using both the microstage and the macrostage models are presented.